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CO2 Capture from Coal fired Power Plants

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Problem Description

Background and objective

There is an increasing interest in CO2 capture and storage as a measure to reduce man-made emissions of the greenhouse gas CO2. Several methods have been proposed for how to do CO2 capture from power plants, both for natural gas and coal. Looking ahead in time, the most abundant fossil fuel source is coal. It is likely that in the long-term (decades), coal will be the main primary energy source globally for generating electricity. The emission of CO2 from coal-fired power plants is in the range 700-1300 g CO2/KWh. This is about 2-3 times that of natural gas fired plants. It is very important to acknowledge the importance of coal and not to think that it is an energy source of the past. For CO2 capture, coal-fired power plants will be very important to focus on, both from the perspective of the amounts of CO2 that will be emitted form such plants, but also from the fact that the CO2 capture cost is low compared to most other large scale technologies, including gas fired power plants. An additional effect of CO2 capture is that in plants where CO2 is to be captured, a number of other pollutants can be or have to be reduced as well.

The main area of this investigation will process modelling and simulations, using a tool like HYSYS or PRO/II. The process to be studied is the IGCC (Integrated Gasification Combined Cycle). This process involves the conversion of the coal energy into a combustible gas that is fed to a gas turbine. The CO2 capture is accomplished as a process step before the combustion of the coal-derived fuel gas.

The project work will be done as cooperation between the two students involved, and only one report is to be written. The work is to be split so that each student has the responsibility of different sub-tasks. However, for the report, with the results, the conclusions and in general quality assurance, both students shall be equally responsible.

One of the candidates shall look into an equilibrium model of coal gasification, and bring that into a general simulation model. This model has to cover a broad variety of coal compositions, and should also cover dry-feed and slurry-feed gasifiers.

The other candidate shall look into modelling of an air separation unit, which purpose is to feed oxygen to the gasifier. The model must cover both low and high-pressure air separation units, as well as LOX and GOX.

Other models, like syngas coolers or quenchers, shift reactors, CO2 capture units, gas turbine and steam turbine modelling will to a large extent be obtained from previous work at NTNU. However, the students shall integrate the sub-models into a total plant model.

The goal of the project is to make a workable model of and IGCC with CO2 capture, that is able to give a detailed heat and mass balance, as well be able to predict sensitivities of various key

Foreword

This master thesis is a co-operation between two master students. The intention was to study a coal fired power plant with CO_2 capture. We think carbon dioxide removal from power production will play a major role in the years to come according to limit human caused global warming. We wanted to learn more about the different processes in a power plant and how to optimize production under a carbon dioxide capture restriction.

The power plant explored and simulated is an Integrated Gasification Combined Cycle (IGCC) power plant. Coal is reacted with steam and oxygen in a partial combustion and CO_2 is removed from the gasified coal before combustion. The main emphasis was placed on simulations of a gasification unit and production of oxygen to the gasifier. In addition the CO_2 capture unit and power island was studied to be get complete IGCC calculations.

To solve the described task a lot of effort were put in studying literature and reports on similar processes. The subjects of gasification and air separation were new to us and the learning curve became steep. We found out that collection of relevant information is difficult due to industry secrets and the fact that there are very few actual IGCC plants in the world.

Through a thorough literature study and computer simulations our understanding of the processes grew. We feel that we have gained a lot of knowledge about IGCC and its involved processes. At the same time we realize that the subject is very wide and to look deeply into every part and every process probably would take a lifetime. In the end we are very satisfied with the finished product.

There are some persons we would like to give credit for helping us completing the thesis. First of all we would like to thank our supervisor professor Olav Bolland and co-supervisor Rahul Anantharaman. Gasification specialist professor Øyvind Skreiberg, MatLab specialist Kjell Kolsaker, Yasser Ahmed at the Simsci helpdesk and the members of Group Bolland has also given us helpful information during the development of the report.

<table>
<tr><td>Esben Tonning Jensen</td><td>Tore Dugstad</td></tr>
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Abstract

Coal is the most common fossil resource for power production worldwide and generates 40% of the worlds total electricity production. Even though coal is considered a pollutive resource, the great amounts and the increasing power demand leads to extensive use even in new developed power plants. To cover the world's future energy demand and at the same time limit our effect on global warming, coal fired power plants with CO_2 capture is probably a necessity.

An Integrated Gasification Combined Cycle (IGCC) Power Plant is a utilization of coal which gives incentives for CO_2 capture. Coal is partially combusted in a reaction with steam and pure oxygen. The oxygen is produced in an air separation process and the steam is generated in the Power Island. Out of the gasifier comes a mixture of mainly H_2 and CO. In a shift reactor the CO and additional steam are converted to CO_2 and more H_2. Carbon dioxide is separated from the hydrogen in a physical absorption process and compressed for storage. Hydrogen diluted with nitrogen from the air separation process is used as fuel in a combined cycle similar to NGCC. A complete IGCC Power Plant is described in this report.

The air separation unit is modeled as a Linde two column process. Ambient air is compressed and cooled to dew point before it is separated into oxygen and nitrogen in a cryogenic distillation process. Out of the island oxygen is at a purity level of 95.6% and the nitrogen has a purity of 99.6%. The production cost of oxygen is 0.238 kWh per kilogram of oxygen delivered at 25°C and 1.4bar. The oxygen is then compressed to a gasification pressure of 42bar.

In the gasification unit the oxygen together with steam is used to gasify the coal. On molar basis the coal composition is 73.5% C, 22.8% H_2, 3.1% O_2, 0.3% N_2 and 0.3% S. The gasification temperature is at 1571°C and out of the unit comes syngas consisting of 66.9% CO, 31.1% H_2, 1.4% H_2O, 0.3% N_2, 0.2% H_2S and 0.1% CO_2. The syngas is cooled and fed to a water gas shift reactor. Here the carbon monoxide is reacted with steam forming carbon dioxide and additional hydrogen. The gas composition of the gas out of the shift reactor is on dry basis 58.2% H_2, 39.0% CO_2, 2.4% CO, 0.2% N_2 and 0.1% H_2S. Both the gasification process and shift reactor is exothermal and there is no need of external heating. This leads to

an exothermal heat loss, but parts of this heat is recovered. The gasifier has a Cold Gas Efficiency (CGE) of 84.0%.

With a partial pressure of CO_2 at 15.7 bar the carbon dioxide is easily removed by physical absorption. After separation the solvent is regenerated by expansion and CO_2 is pressurized to 110bar to be stored. This process is not modeled, but for the scrubbing part an energy consumption of 0.08kWh per kilogram CO_2 removed is assumed. For the compression of CO_2, it is calculated with an energy consumption of 0.11kWh per kilogram CO_2 removed. Removal of H_2S and other pollutive unwanted substances is also removed in the CO_2 scrubber.

Between the CO_2 removal and the combustion chamber is the H_2 rich fuel gas is diluted with nitrogen from the air separation unit. This is done to increase the mass flow through the turbine. The amount of nitrogen available is decided by the amount of oxygen produced to the gasification process. Almost all the nitrogen produced may be utilized as diluter except from a few percent used in the coal feeding procedure to the gasifier. The diluted fuel gas has a composition of 50.4% H_2, 46.1% N_2, 2.1% CO and 1.4% CO_2.

In the Power Island a combined cycle with a gas turbine able to handle large H_2 amounts is used. The use of steam in the gasifier and shift reactor are integrated in the heat recovery steam generator (HRSG) in the steam cycle. The heat removed from the syngas cooler is also recovered in the HRSG.

The overall efficiency of the IGCC plant modeled is 36.8%. This includes oxygen and nitrogen production and compression, production of high pressure steam used in the Gasification Island, coal feeding costs, CO_2 removal and compression and pressure losses through the processes. Other losses are not implemented and will probably reduce the efficiency.

Sammendrag

Kull er den mest utbredte fossile ressursen for kraftproduksjon i verden og står for 40% av verdens elektrisitetsproduksjon. Selv om kull er betraktet som en forurensende ressurs, medfører den store tilgjengeligheten samt verdens økende energibehov til utstrakt bruk også i nye kraftverk. For å dekke verdens fremtidige energibehov samtidig som vår påvirkning på global oppvarming begrenses, er kullkraftverk med CO_2 innfangning sannsynligvis en nødvendighet.

Et Integrated Gasification Combined Cycle (IGCC) kraftverk er en utnyttelse av kull som gir insentiver for CO_2 innfangning. Kull reagerer med damp og rent oksygen i en partiell forbrenning. Oksygen er fremstillet i en luftseparasjonsprosess og dampen er produsert i kraftsyklusen. Etter gassifiseringen er brenselet en blanding av hovedsakelig H_2 og CO. I en shift reaktor er CO og tilført damp konvertert til CO_2 og mer H_2. Karbondioksid blir skillet fra hydrogenet i en fysisk absorpsjonsprosess og komprimert for lagring. Hydrogen fortynnet med nitrogen fra luftseparasjonsprosessen er brukt som brensel i en kombinert gass- og dampsyklus tilsvarende som for gasskraftverk. Et komplett IGCC anlegg er presentert i denne rapport.

Luftseparasjonsenheten modellert tilsvarer Lindes dobbel-kolonne prosess. Luft er komprimert og kjølnet til duggpunkt før den er separert til oksygen og nitrogen i en kryogenisk destillasjonsprosess. Ut av enheten kommer oksygen med en renhet på 95.6% og nitrogen med en renhet på 99.6%. Oksygenets produksjonskostnad er på 0.238kWh per kilogram oksygen levert ved 25°C og 1.4bar. Oksygenet er deretter komprimert til et gassifiseringtrykk på 42bar.

I gasifiseringsenheten er oksygen brukt sammen med damp til å gassifisere kull. Kullet har på molar basis følgende sammensetning, 73.5% C, 22.8% H_2, 3.1% O_2 og 0.3% av henholdsvis N_2 og S. Gasifiseringen skjer ved 1571°C og ut av prosessen kommer syngas bestående av 66.9% CO, 31.1% H_2, 1.4% H_2O, 0.3% N_2, 0.2% H_2S and 0.1% CO_2. Gassen er kjølnet og sendt til en shift reaktor. Her reagerer karbonmonoksidet med damp og danner karbondioksid og hydrogen. Sammensetningen av gassen ut av shift reaktoren er på tørr basis 58.2% H_2, 39.0% CO_2, 2.4% CO, 0.2% N_2 og 0.1% H_2S. Både gasifiserings- og shiftprosessen er

eksoterme og har ikke behov for ekstern varmetilførsel. Dette fører til et eksotermt varmetap, men deler av varmen er gjenvunnet. Gasifiseringsprosessen har en gasifiseringsvirkningsgrad (CGE) på 84.0%.

Med et partielltrykk på 15.7bar er det relativt enkelt å skille CO_2 fra brenselsgassen ved fysisk absorpsjon. Etter separasjonen er løsningsmiddelet regenerert ved ekspansjon og karbondioksidet er komprimert til lagringstrykk på 110bar. Denne prosessen er ikke modellert, men for utskillelsesprosessen er det antatt et energiforbruk på 0.08kWh per kilogram CO_2 fjernet. For kompresjonsarbeidet er det regnet med et energiforbruk på 0.11kWh per kilogram CO_2 fjernet. Innfangning av H_2S og andre forurensende uønskede stoffer er også fjernet i denne enheten.

Mellom CO_2 fjerningen og brennkammeret er den hydrogenrike brenselsgassen fortynnet med nitrogen fra luftseparasjonsenheten. Dette er gjort for å øke massestrømmen gjennom turbinen. Mengden tilgjengelig nitrogen er bestemt av oksygenbehovet i gasifiseringsenheten. Sett bort fra et par prosent nitrogen brukt i fødeprosedyren for kull til gasifiseringsenheten, kan all nitrogenet brukes som brenselsgassfortynner. Den fortynnede brenselsgassen har følgende sammensetning, 50.4% H_2, 46.1% N_2, 2.1% CO og 1.4% CO_2.

I kraftprosessen er det brukt en gassturbin som håndterer høyt innhold av hydrogen i brenselet. Bruken av damp i gasifiserings- og shiftprosessen er integrert i Heat Recovery Steam Generatoren (HRSG) i dampsyklusen. Varmen fjernet i syngaskjølingen er også gjenvunnet i HRSG.

Den totale virkningsgraden for IGCC kraftverket modellert er på 36.8%. Dette inkluderer oksygen og nitrogen produksjon og kompresjon, produksjon av høytrykks damp brukt i gasifiseringen, kullfødekostnader, CO_2 innfangning og kompresjon og trykktap gjennom prosessene. Andre tap er ikke medregnet og vil sannsynligvis redusere virkningsgraden ytterligere.

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Abbreviations

AGR	Acid Gas Removal
Ar	Argon
ASU	Air Separation Unit
CCP	Clean Coal Power
CCR	Combined Condenser and Reboiler
CCS	Carbon Capture and Storage
CFZ	Controlled Freezing Zone
CGE	Cold Gas Efficiency
CO	Carbon monoxide
CO_2	Carbon dioxide
COS	Carbonyl sulfide
DEMEA	Type of Monoethanolamine
EOR	Enhanced Oil Recovery
GE	General Electric
GOX	Gaseous Oxygen
GT	Gas turbine
H_2	Hydrogen
H_2S	Hydrogen sulfide
HCN	Hydrogen cyanide
HP	High Pressure
HRSG	Heat Recovery Steam Generator
IEA	International Energy Agency
IGCC	Integrated Gasification Combined Cycle
IPCC	Intergovernmental Panel on Climate Change
KT	Koppers-Totzek
LHV	Lower Heating Value
LOX	Liquid Oxygen
LP	Low Pressure
N_2	Nitrogen
NGCC	Natural Gas Combined Cycle
O_2	Oxygen
PPU	Pre Purification Unit
SCGP	Shell Coal Gasification Process
ST	Steam turbine
TIT	Turbine Inlet Temperature
WGS	Water gas shift reaction
ΔT	Minimum Temperature Approach

1 Introduction

1.1 CO$_2$ emissions

The issue of global warming has been discussed by scientists for 30 years without affecting the public remarkable. The registered increase in temperature the last 50 years has been explained by either natural temperature oscillations or man made greenhouse gas emissions. In the last 10 years the relationship between greenhouse gases and global warming has become a wide agreement among scientists. In 1997 the Kyoto Protocol was negotiated with a common goal of the governments ratified the treaty of "achieving stabilization of greenhouse gas concentrations in the atmosphere at a level that would prevent dangerous anthropogenic interference with the climate system" [1].

The climate change is today admitted as a problem by almost every scientist, state leader and random man. According to a conservative assumption by the IPCC there is a 90 percentage possibility that the global warming originates from man made greenhouse gas emissions [2].

The major greenhouse gas emitted by humans is carbon dioxide. Carbon dioxide is a natural end product in all kind of combustions from fossil fuel fired power plants to sparkling firewood in the fireplace. Carbon in wood, natural gas, oil or coal reacts with oxygen and forms carbon dioxide and water vapor.

Power production is one of the largest contributors to CO_2 emissions. Combustion of coal, oil or natural gas to produce heat and electricity leads to great emission rates of carbon dioxide. The amount of CO_2 emitted varies with type of fuel and combustion technology. Carbon rich fuels like coal produce most CO_2 per amount of energy while hydrogen rich fuels like natural gas have smaller emissions. In this case it is advantageous to look at the m over n ratio, where m is carbon and n is hydrogen. Under equal combustion criteria a higher m over n ratio leads to higher CO_2 emissions.

$$\left(\frac{m}{n}\right)_{coal} > \left(\frac{m}{n}\right)_{oil} > \left(\frac{m}{n}\right)_{natural\,gas} \quad \Rightarrow \quad (\approx 1.1)_{coal} > (\approx 0.5)_{oil} > (\approx 0.25)_{natural\,gas} \qquad (1.1)$$

Combustion of coal leads to a remarkable higher emission rate than oil or natural gas. The exhaust gas from coal combustion contains 12-14 percent carbon dioxide while exhaust gas from natural gas only contains 3.2-4.2 percent. In amounts this equals to 750-1100 gram per kilowatt hour of electricity produced in a coal fired power plant compared to 300-350 gram in a natural gas fired power plant [3] [4].

Although, the great coal resources gives coal a significant role in covering the increasing global energy demand. And to reduce the worlds total carbon dioxide emissions the reduction must be done where it matters, combustion of carbon rich fuels.

1.2 Coal fired Power Plants

This report focuses at coal fired power plants. Coal is the fossil fuel there is most of in the world and it will be one of the main resources for power production in many years to come. According to BP statistics the world need of coal is covered for 147 years [5]. To satisfy both the increasing energy demand and the goal of the Kyoto Protocol the technology in the coal fired power plants need to be improved.

Conventional coal fired power plants use a Rankine cycle to transform the coal into power. A Rankine cycle is simplified shown in figure 1.1.
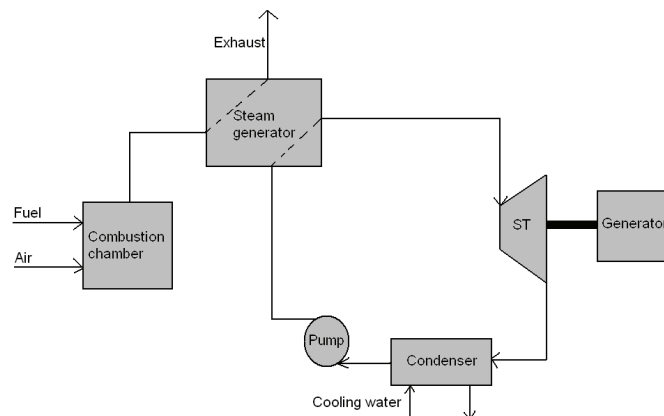
Figure 1.1. Rankine cycle.

The most efficient power plants based on a Rankine cycle is the Pulverized Coal (PC) plant. The combustion of the pulverized coal produces exhaust gas which contains CO_2 that may be captured.

In this report a newer and more modern way to combust coal is studied. It is called an Integrated Gasification Combined Cycle power plant and there are per today only 3 or 4 commercial IGCC plants in the world [6]. The idea of an IGCC plant is to transform the coal into a gas which can be utilized like natural gas in a combined cycle. Figure 1.2 shows an overview of a combined cycle.
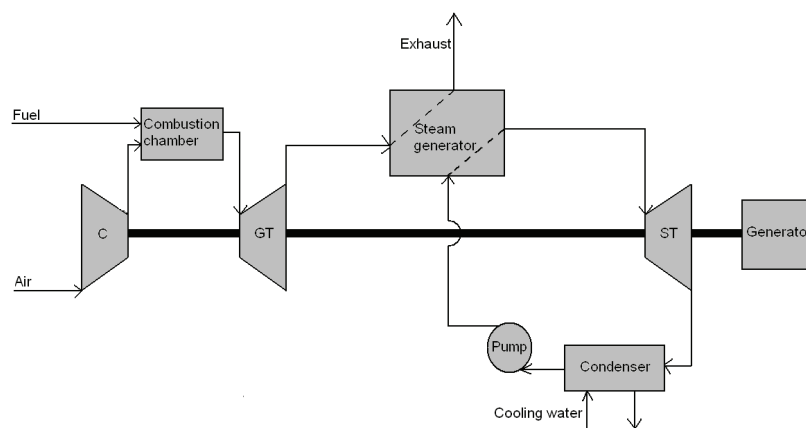
Figure 1.2. Combined cycle, Brayton and Rankine.

The CO_2 capture is done before the combustion. This is done by transforming the coal into a gas consisting of mainly CO_2 and H_2. The two gases are separated and the CO_2 is sent to storage while the H_2 is used as fuel in the combined cycle.

The advantage of IGCC is an energy cost reduction in the CO_2 removal unit. According to IPCC a new coal fired power plant without CO_2 capture has a higher efficiency built as a PC plant than an IGCC plant. With implementation of a CO_2 removal demand, the relative low capture cost in the IGCC plant gives higher efficiency for an IGCC than a PC. Efficiencies are given in table 1.1.

Table 1.1. Energy efficiency in coal fired power plants [2].

	New PC plant	New IGCC plant
Plant efficiency without CO2 capture, LHV basis (%)	48	43
Plant efficiency with CO2 capture, LHV basis (%)	33	35

The efficiency in each case may have some variations with surrounding conditions and different technologies.

Table 1.1 shows that for plants with capture of carbon dioxide IGCC has a higher efficiency and is probably a more future oriented type of power plant.

1.3 Integrated Gasification Combined Cycle

The integrated gasification combined cycle consists of 4 main processes, the air separation island, the gasification island, the acid gas removal and the power island. Figure 1.3 shows a block diagram of an IGCC plant with color separation between the four main processes.
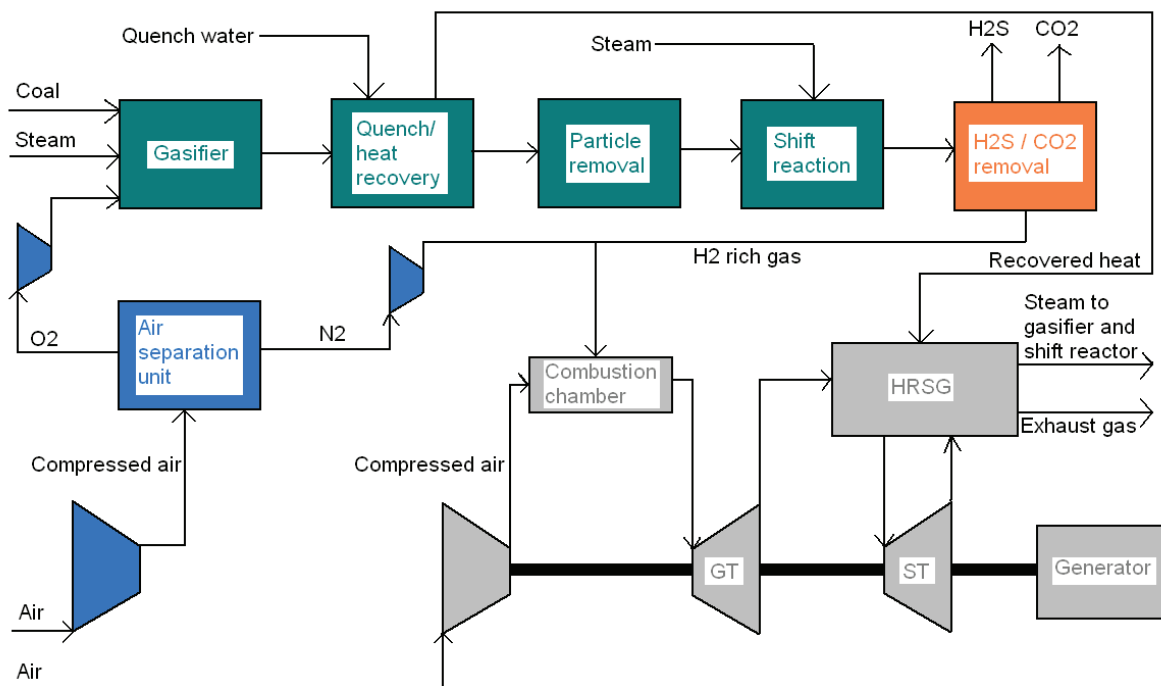
Figure 1.3. Overview of the main processes in an IGCC Power Plant.

In the Air Separation Island air is separated into oxygen and nitrogen. The oxygen is used together with steam and coal in the Gasification Island. Out of the Gasification Island a gas consisting mainly of hydrogen and carbon dioxide is sent to the acid gas removal facility. Here the CO_2 and the traces of H_2S in the gas are separated from the hydrogen. H_2S and CO_2 are sent to further treatment and storage while the hydrogen rich gas is mixed with nitrogen

from the air separation unit before entering the combustion chamber. In the Power Island electricity is generated similar to the power cycle in a natural gas fired power plant.

This report is chronological studying these four main processes in detail. The theory behind each process is presented before simulations and calculations are made for each island. In the end the islands are set together in a complete IGCC Power Plant model.

2 Theoretical Background

2.1 Air Separation Island

2.1.1 Distillation theory

A distillation column separates two or more components based on the different boiling points for the given substances. The special case of air separation for an IGCC plant is principally to separate oxygen and nitrogen. In addition to oxygen and nitrogen, air also contains argon, water, carbon dioxide and traces of other substances. The traces are normally neglected while the water and the CO_2 should be removed before the distillation column. It is also a question if the argon should be separated from oxygen and nitrogen or not. If the argon can be utilized it may be economical beneficial to remove it.

There are several factors that influence the performance of a distillation column. The feed rate and the feed content play a major role and will affect the design of the column. The main property of this is the boiling point of the different substances. Small differences in boiling point require a more advanced separation process. In the case of N_2 and O_2 the difference in boiling point at 1 atmosphere is about 13˚C [7]. Argon has boiling point between oxygen and nitrogen and removal of argon therefore complicates the process. Roughly spoken, the wanted purity of the products (degree of separation) determines the height of the column while the amount of feed determines the diameter [8].

In this part of the report a theoretical introduction to distillation is given. Sources for the derivations are Humphrey [8] and Geankoplis [9]. In chapter *2.1.2 Air Separation Unit* the specific case of oxygen-nitrogen separation is further explained.

2.1.1.1 Equilibrium

Equilibrium between liquid and vapor phase is reached when no further changes in composition, temperature or pressure occur in a fixed environment. A typical distillation

column contains a lot of steps or trays where equilibrium conditions occur. A single step may be studied as a tank where an external heat source heats the contents and boiling will occur. The most volatile component will concentrate more in vapor phase while the component with higher boiling point will concentrate in liquid phase. In a column with many trays the vapor will move upwards to the next stage, reach å new equilibrium with the down coming liquid and so on. Likewise the liquid will move downwards and meet the upcoming vapor. The vapor purity at the top of the column depends on the number of equilibrium trays. This is likewise for the liquid in the bottom.

The equilibrium ratio is defined from equation 2.1.

$$K_i = \frac{y_i}{x_i} \tag{2.1}$$

K_i is the equilibrium ratio, y_i is the molar fraction of component *i* in vapor phase and x_i is the molar fraction of component *i* in liquid phase.

A component with low boiling point will have a higher equilibrium ratio than a less volatile component. The K-value is used to determine the separation factor between two substances. This is known as relative volatility and the definition is shown in equation 2.2.

$$\alpha_{ij} = \frac{K_i}{K_j} \tag{2.2}$$

Substituting equation 2.1 into 2.2 gives equation 2.3.

$$\alpha_{ij} = \frac{y_i / x_i}{y_j / x_j} = \frac{y_i / x_i}{(1 - y_i)/(1 - x_i)} \tag{2.3}$$

Equation 2.3 can be rearranged to 2.4.

$$y_i = \frac{\alpha_{ij} x_i}{1 + (\alpha_{ij} - 1)x_i} \tag{2.4}$$

Equation 2.4 shows the vapor fraction as a function of liquid fraction and relative volatility. This relation is often presented graphical.

With ideal equilibrium conditions Raoult's law may be derived.

$$p_i = P_i^\circ x_i \tag{2.5}$$

In equation 2.5 is p_i the partial pressure of component i in the vapor while P_i° is the vapor pressure of pure component i. The vapor pressure is tabulated for different substances and x_i is the molar fraction of component i in the liquid.

Another ideal law for systems of vapor and liquid is the Dalton's law.

$$p_i = P y_i \tag{2.6}$$

Here is P the total pressure. Equation 2.6 can be rearranged and combined with equation 2.5.

$$y_i = \frac{p_i}{P} = \frac{P_i^\circ x_i}{P} \tag{2.7}$$

The same is legal for component j and using y_i and y_j in equation 2.3 gives 2.8 gives.

$$\alpha_{ij} = \frac{y_i / x_i}{y_j / x_j} = \frac{\dfrac{P_i^\circ x_i}{P} \bullet \dfrac{1}{x_i}}{\dfrac{P_j^\circ x_j}{P} \bullet \dfrac{1}{x_j}} = \frac{P_i^\circ}{P_j^\circ} \tag{2.8}$$

From equation 2.8 the separation potential for two substances may be determined. α_{ij} is decided and through equation 2.4 the vapor fractions may be plotted against the liquid fractions. Equation 2.8 gives the α_{ij} - value for ideal conditions. For non ideal systems the behavior is corrected with an activity coefficient γ. The expression for the relative volatility under non ideal conditions is given in 2.9.

$$\alpha_{ij} = \frac{\gamma_i P_i^\circ}{\gamma_j P_j^\circ} \tag{2.9}$$
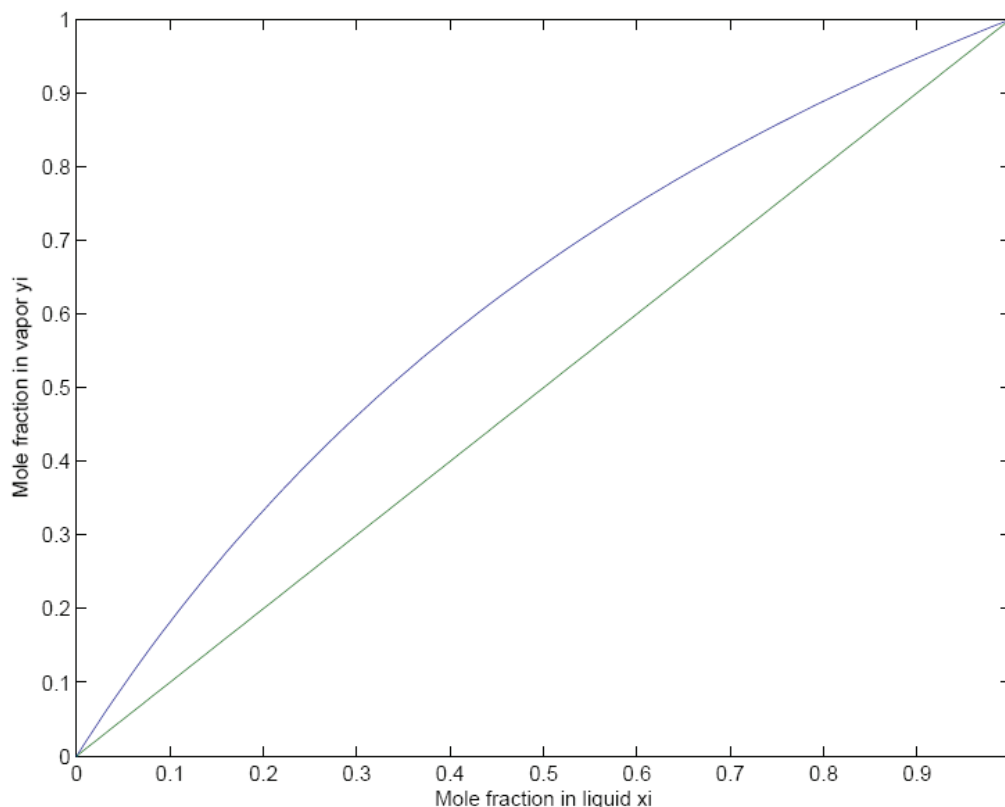
Figure 2.1. Vapor – liquid separation.

Figure 2.1 shows the vapor fractions as a function of liquid fractions and relative volatility. The 45 degree line y=x indicates the situation of no separation which is similar to a α_{ij}-coefficient equal 1. A high α_{ij} value bends the other line away from y=x and eases the separation.

2.1.1.2   McCabe-Thiele Method

Figure 2.2 gives an overview of a distillation column including a reboiler and a condenser. The Feed (F) is in this example fed in the middle of the column and the vapor phase is enriching in upwards direction. A condenser is installed at the top to condensate some of the outgoing product and send it back to the column to improve efficiency. The amount of top product going back to the column is called reflux and decided by the operator. The rest is moved away from the column as distillated product. From this the quality or purity of the distillate can be specified. The ratio between the distillate (D) and the reflux stream (L_0) is called the reflux ratio R, and is defined by 2.10.

$$R = \frac{L_0}{D} \tag{2.10}$$

The reflux ratio is important in calculations regarding to the energy consumption in the distillation column.
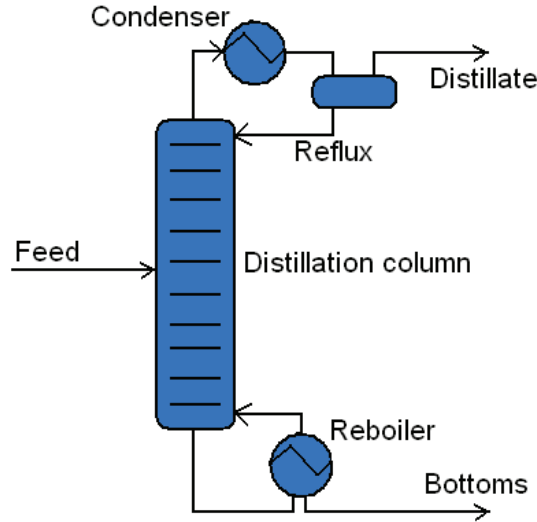
Figure 2.2. Distillation column with condenser and reboiler.

At the bottom there is a reboiler with similar purpose as the condenser. The bottom product (B) out of the reboiler is in liquid phase and the feed back to the column is in vapor phase. The operational specifications in the reboiler can similar to the condenser specify the purity of the bottom product. In air separation, the Linde process with two columns is normally utilized. Heat transfer between the columns is then implemented to improve efficiency. This is explained in detail in *2.1.2.7 Combined condenser and reboiler*.

The section over the feed stream is called the rectifier section while the section under the feed is called the stripping section. These two sections will be studied separately as a part of a complete investigation of the column.

A material balance for the column is given by equation 2.11.

$$F = D + B \tag{2.11}$$

The feed (F), distillate (D) and the bottoms (B) are defined as molar flows. Likewise a material balance for one component can be derived.

$$Fx_F = Dx_D + Bx_B \tag{2.12}$$

x is the concentration of the most volatile component respectively for feed, distillate and bottom.

Rectifier section

Figure 2.3 shows the upper part of a distillation column called the rectifier section.
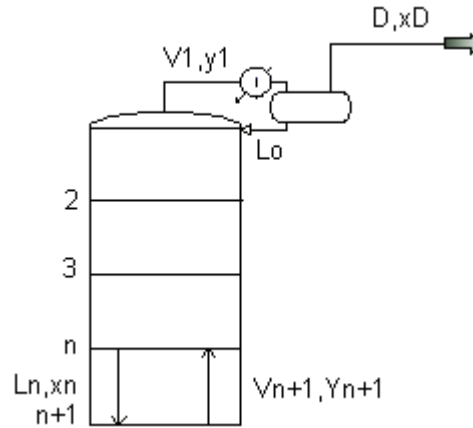
Figure 2.3. Rectifier section.

At stage n+1, V_{n+1} flows upward in vapor phase. All the up going flow must either be removed as distillate or go back to the column in liquid phase as reflux L_0. One can assume equal molar flow which gives the connections, $L_2=L_3=L_n$ and $V_2=V_3=V_n=V_{n+1}$. Based on the assumptions of equal molar flow there can be made an overall material balance for the rectifier part.

$$V_{n+1} = L_n + D \qquad (2.13)$$

For one component, the up flowing and most volatile component, the material balance is expressed by equation 2.14.

$$V_{n+1}y_{n+1} = L_n x_n + Dx_D \qquad (2.14)$$

y_{n+1}, x_n and x_D are respectively the molar fraction of vapor at stage n+1, of liquid at stage n and finally the molar fraction of the distillate product.

Equation 2.14 can be rearranged to solve y_{n+1} as a function of x_n and x_D.

$$y_{n+1} = \frac{L_n}{V_{n+1}}x_n + \frac{D}{V_{n+1}}x_D \qquad (2.15)$$

Rearranging equation 2.15 and using the definition of reflux ratio from equation 2.10 gives equation 2.16 and 2.17.

$$\frac{D}{V_{n+1}} = \frac{1}{R+1} \tag{2.16}$$

$$\frac{L_n}{V_{n+1}} = 1 - \frac{D}{V_{n+1}} = 1 - \frac{1}{R+1} = \frac{R}{R+1} \tag{2.17}$$

Equation 2.16 and 2.17 put into equation 2.15 gives the equation for the enriching part given in 2.18.

$$y_{n+1} = \frac{R}{R+1}x_n + \frac{1}{R+1}x_D \tag{2.18}$$

This relation can be plotted in a liquid vapor diagram and it will occur as a straight line for constant reflux ratio.

Stripping section

Figure 2.4 shows the lower part called the stripping section. At stage m+1 liquid L_m flows downwards while vapor V_{m+1} goes upward in the same way as for the rectifier section.
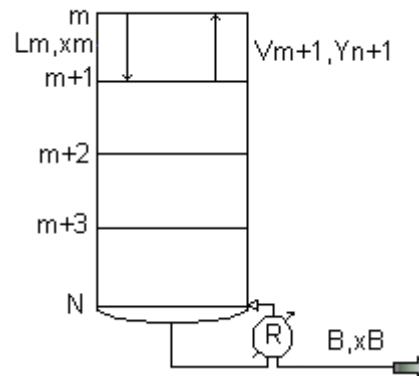
Figure 2.4. Stripping section.

With equal assumption as for the top of the column a total material balance is given in 2.19.

$$V_{m+1} = L_m - B \tag{2.19}$$

The most volatile components material balance is given in equation 2.20.

$$V_{m+1}y_{m+1} = L_m x_m - B x_B \tag{2.20}$$

y_{m+1}, x_m and x_B are still molar fraction in respectively vapor and liquid phase. Equation 2.20 is rearranged for plotting and solving y_{m+1} as a function of x_m and x_B.

$$y_{m+1} = \frac{L_m}{V_{m+1}} x_m - \frac{B}{V_{m+1}} x_B \qquad (2.21)$$

Equation 2.18 and 2.21 present the operating line for the rectifier and the stripping section. The pitch line between these sections is the feed stream. The section over the feed stream is the rectifier part while the portion below the feed stream is the stripping section. The location of the feed is determined by the condition of the feed stream, mainly the thermal condition expressed in equation 2.22.

$$q = \frac{H_V - H_F}{H_V - H_L} \qquad (2.22)$$

H_V is the enthalpy of the feed at the dew point, H_L is the enthalpy of the feed at the boiling point and H_F is the enthalpy of the incoming feed. Equation 2.22 expresses the heat required to vaporize 1 mol of feed compared to vaporize 1 mol of liquid feed. The value of q describes the conditions. If the feed enters as liquid at boiling point $H_F=H_L$ and the q value is 1. If the feed enters as vapor at dew point $H_V-H_F=0$ and $q=0$. $q>1$ means that the feed enters as a sub cooled liquid and $q<0$ indicates a superheated vapor feed stream. The typical situation of q value is between 0 and 1, part liquid, part vapor.

A material balance using q may now be set up. Figure 2.5 shows a tray overview at the feed tray. qF gives the liquid part of the feed and *(1-q)F* gives the vapor part.
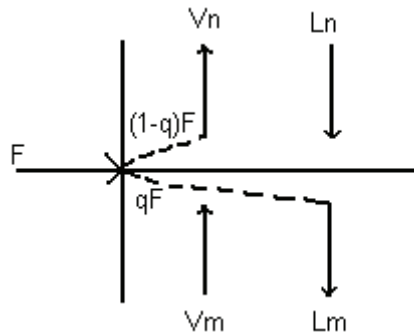
Figure 2.5. Feed tray.

Material balances can be made for the liquid and the vapor phase using the q relations.

$$L_m = L_n + qF \tag{2.23}$$

$$V_n = V_m + (1-q)F \tag{2.24}$$

Equation 2.14 and 2.20 can be rewritten to 2.25 and 2.26.

$$V_n y = L_n x + Dx_D \tag{2.25}$$

$$V_m y = L_m x - Bx_B \tag{2.26}$$

Subtracting equation 2.25 from 2.26 gives 2.27.

$$(V_m - V_n)y = (L_m - L_n)x - (Dx_D + Bx_B) \tag{2.27}$$

Rearranging this for y versus x gives equation 2.28.

$$y = \frac{(L_m - L_n)}{(V_m - V_n)}x - \frac{(Dx_D + Bx_B)}{(V_m - V_n)} \tag{2.28}$$

In addition one may include the overall balance $Dx_D + Bx_B = x_F$ and B17 is rewritten to 2.29.

$$y = \frac{q}{q-1}x - \frac{1}{q-1}x_F \tag{2.29}$$

The latest equation is called the *q-line* equation. This represents the location of the intersection between the enriching and stripping line. The connection between the equilibrium line given by equation 2.4, the enriching line given 2.18, the stripping line given by 2.21 and the q-line given by 2.29, is drawn in figure 2.6.

The equations derived here is the theoretical fundament for air separation. The rest of this report will focus in a more practical direction in the way of modeling and simulations.
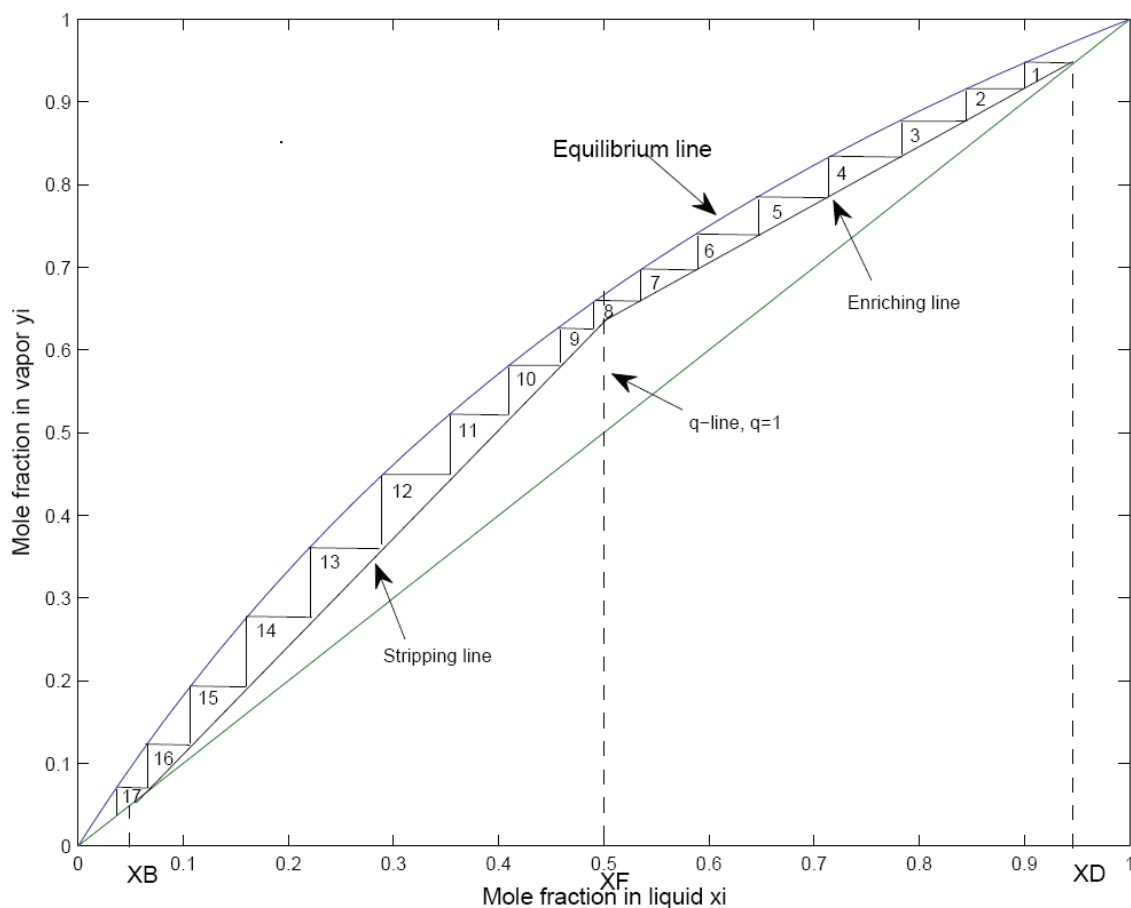
Figure 2.6. McCabe Thiele diagram.

The dashed lines $y=x_B$ and $y=x_D$ shows the wanted purity in bottoms and distillate while $y=x_F$ gives the liquid fraction in the feed. The shape of the q-line is here for a q-value equal to 1. The q-line will always start at the intersection between $y=x_F$ and the 45° line and turned to left or right dependent on the feed. To determine the border between the enriching and stripping zone the enriching line is first drawn together with the q-line. The intersection of those lines is the starting point for the stripping line. The "stairs" indicates the number of theoretical trays for the given column with the given properties.

2.1.2 *Air separation unit*

2.1.2.1 Introduction

The objective of an air separation unit, ASU, is to convert ambient air to pure oxygen and pure nitrogen. Normally oxygen is the needed outcome, but in many cases the inert nitrogen also has a utility value. In air separation for gasification, oxygen is the only utilized product from the ASU. Although when the gasification is done for power production the nitrogen is important to dilute the fuel entering the power cycle. In IGCC both oxygen and nitrogen from the air separation unit is used in the subsequent Gasification Island and Power Island.

An air separation unit may be seen as a cooling machine. Air is compressed, cooled and choked to remove heat from the cycle. This is done in a temperature area and a pressure level which leads to liquefied oxygen. The oxygen and nitrogen is separated in a set of distillation columns. The energy cost of separating oxygen and nitrogen is put on the compression work of the air compressor. Mature air separation technologies produce oxygen at an energy cost of about 0.22 to 0.25 kWh per kilogram pure oxygen [10]. Figure 2.7 shows an overview of an Air Separation Island.

Figure 2.7. Air separation unit.

Figure 2.7 shows a conventional gaseous oxygen (GOX) production plant. When oxygen is needed at a high pressure it is possible to lower the energy cost with 1-2 percent with a liquid oxygen (LOX) production plant [7]. The differences between GOX and LOX production are small and GOX production is first presented before the differences are pointed out in *2.1.2.10 Liquid oxygen.*

Ambient air is fed to the main air compressor and compressed to a pressure level at 5-7bar [10]. The air stream is cooled back to ambient temperature and fed to a molecular sieve for removal of moisture and carbon dioxide. In the main heat exchanger the air is cooled to a temperature near dew point before it is fed to the high pressure (HP) column. The column separates the air into two streams, an almost pure nitrogen stream in the top and an oxygen rich stream in the bottom. The nitrogen stream is cooled further, chocked to a lower pressure and fed to the top tray of the low pressure (LP) column. The oxygen stream is choked and fed about in the middle of the low pressure column. Out of the low pressure column a pure nitrogen stream is taken out in the top and a pure oxygen stream is taken out in the bottom. These streams are very cold and are used to cool other parts of the island. Out of the main heat exchanger the nitrogen and oxygen streams are at ambient temperature and at a pressure level slightly above atmospheric.

In ASU design, it is important to focus on the outcome of the island. As mentioned, the goal is to produce pure oxygen and nitrogen. There will always be traces of other substances in a so called pure gas and one of the main decisions in the design process is to decide the required purity. It is normal to have oxygen purity between 95 and 99.9 percent dependent on the subsequent application and the cost of increased purity. For gasification purpose a purity of 95 percent is tolerable [11]. In IGCC nitrogen is diluting the fuel before the power island. To avoid reaction between oxygen in the nitrogen stream and the fuel before the combustion chamber a nitrogen purity of 99 percent is demanded [7].

Each of the processes mentioned in the introduction will in the subsequent chapters be closer explained.

2.1.2.2 Compression

At the compressor inlet the air is at ambient conditions. The main air compressor is in real life a set of several smaller compressors in series. The number of compressors varies with compression rate and is a question of investment costs versus operating costs. Many compressors with low lifting height on each compressor give lower operating costs, but larger investment expenses. On the other hand are fewer compressors with larger lifting heights cheaper to buy, but demands a larger energy input.

Typical operating pressure for the high pressure column is 5 to 7 bar [11]. The outlet pressure at the last compressor must be at a level which includes pressure losses in the subsequent units. This must be done to feed the high pressure column at the wanted pressure.

After compression the air is cooled to a near ambient temperature. The separation island is a sort of cooling machine and it is advantageous to cool the air as much as possible before the main heat exchanger. The air cooling after the main compressor is done after each compression step. The energy demand for compression of cold air is lower than for hot air and air cooling between each step therefore leads to a lower total energy input.

Cooling of the air gives a 2-3 percent pressure loss in each aftercooler, but decreased energy consumption for compression of colder air makes it favourable [10].

2.1.2.3 Air cleaning

Before the compressed air enters the main heat exchanger it has to be dried and cleaned. Even though air mainly consists of nitrogen and oxygen, a small amount of water vapor, argon and carbon dioxide needs to be taken into account. In addition there are traces of various other substances, but the amounts of these can be neglected. Table 2.1 gives the composition of 1 atmosphere, 15°C [12].

Table 2.1. Dry air at 1 atmosphere, 15°C [12].

Component	Volume percent
N_2	78.084
O_2	20.948
Ar	0.934
CO_2	0.031
Other	0.003

The amount of water vapor in the air is dependent of the humidity in the air. This is again dependent on time and location of where the air inlet is placed. A typical assumption is to calculate with a water amount of one percent in moist air. Table 2.2 shows the adjusted composition of air containing 1 percentage of H_2O.

Table 2.2. Moist air at 1 atmosphere, 15°C.

Component	Volume percent
N_2	77.303
O_2	20.739
H_2O	1.000
Ar	0.925
CO_2	0.030
Other	0.003

The traces of other substances listed in table 2.1 and 2.2 are for most cases neglected.

Before entering the first distillation column, water vapor and carbon dioxide must be removed from the air mixture. At the operating conditions in the units, water and CO_2 will freeze and disturb proper work of the columns.

Water vapor may easily be removed by condensation in the heat exchanger. Carbon dioxide is on the other hand not easily removed by condensation. This is because of the condensation temperature of CO_2 is very close to the condensation temperature of O_2 [13]. CO_2 removal by condensation demands a very accurate operating heat exchanger. This technology is called reversing heat exchangers. CO_2 and water vapor condensates and freezes onto the walls in the heat exchanger. The heat exchanger used is the main heat exchanger. From time to time the duty of the heat exchanger is reversed and the frozen CO_2 and water evaporate and are sent

back to the atmosphere in a waste gas stream. This technology demands a production stop every time the heat exchanger is cleaned for frozen waste products and is therefore not optimal for large scale units [14].

The solution for large scale air separators is to use a molecular sieve pre purification unit (PPU) to remove both water vapor and carbon dioxide. The molecular sieves remove water vapor and CO_2 by adsorption at near ambient conditions. A molecular sieve typically contains of two vessels where one of the vessels is used to purify the air and the other vessel is being regenerated. The advantage of molecular sieves is the ability to operate at stationary conditions with no need for production stop. If the air separation island is located in an environment with air containing other unwanted components, a molecular sieve can normally be designed to handle these challenges [14].

After removal of CO_2 and water vapor the air is sent to the main heat exchanger.

2.1.2.4   Main heat exchanger

In the main heat exchanger air is cooled to a temperature near dew point for the given pressure. The oxygen and nitrogen streams from the low pressure column are used as cold streams in this process. The airflow into main heat exchanger equals the sum of the O_2 and the N_2 stream out of the exchanger since there is no other inlets or outlets in the air separation unit. An overview of the in and outgoing flows in the main heat exchanger is shown in figure 2.8.
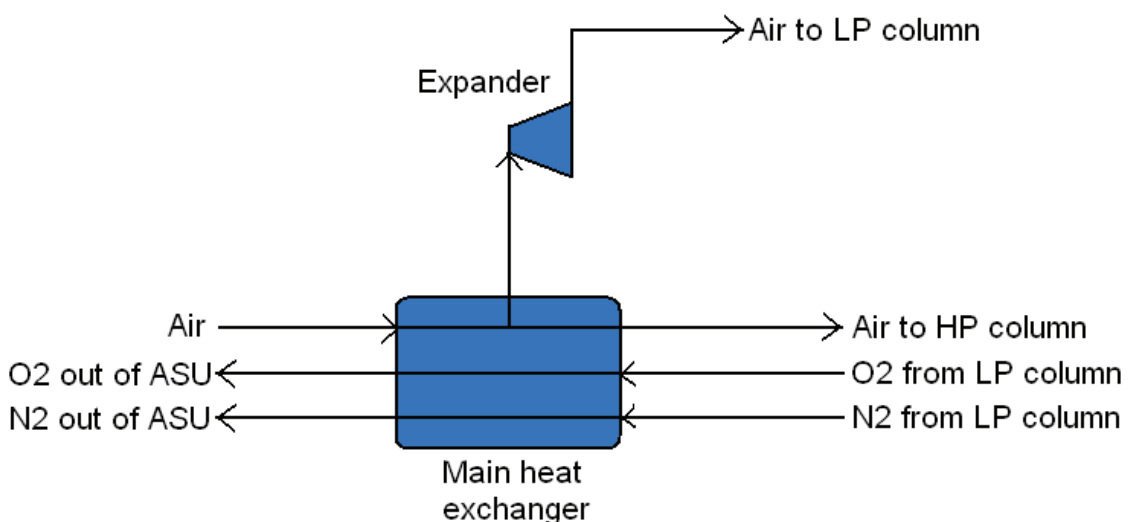
Figure 2.8. Main heat exchanger.

As mentioned in *2.1.2.1 Introduction,* an air separation unit may be considered as a cooling machine. Coldness is produced by compression with aftercooling to near ambient temperature and choking to achieve temperatures below ambient.

Compression work is the only external energy input to the air separation island. The cold needed in the unit must be produced by compression, heat exchanging and choking. If there is an increased demand of coldness, if for example the island is a LOX island instead of a GOX island, the extra heat removal is produced by a booster compressor with heat exchanging in the main heat exchanger and choking afterwards. This is closer explained in *2.1.2.10 Liquid oxygen.*

In this heat exchanger a small amount of air is taken out in the exchanger and led to the low pressure column. This is done to have enough heat in the in the combined condenser and reboiler between the columns. This is also explained in section *2.1.2.7 Combined condenser and reboiler*. The amount of air sent to the low pressure column is about 10 percent of the airflow [7].

When designing a heat exchanger an economic consideration about the conduction ability is required. Heat exchangers with high conduction rates are expensive, but in units with small temperature differences, like air separators, they are necessary. Due to low temperature differences in the streams there is no room for low conduction rates. ΔT is the value showing this minimum temperature difference between hot inlet temperature and cold outlet temperature, and cold inlet temperature and hot outlet temperature, there can be in a heat exchanger. ΔT is called minimum temperature approach. A low ΔT gives high conduction ability, but the heat exchanger is expensive. A high ΔT gives lower conduction ability, but on the other hand the exchangers are cheaper to buy [15]. As mentioned, air separators normally have low temperature difference and therefore demands high quality heat exchangers with a low ΔT. Typical ΔT for exchangers in air separation units are 1-2K [10].

After the main heat exchanger is air at a temperature near dew point for the given pressure sent to the high pressure column. Pure nitrogen and oxygen are sent out of the air separation unit to pre treatment.

2.1.2.5   High pressure column

The LP column has a condenser, but no reboiler. The pressurized, cleaned, cold air is fed to the bottom tray of the column. Almost pure nitrogen comes out of the condenser and is sent to the low pressure column. Out of the bottom of the column an oxygen rich gas is sent. An overview of the high pressure column is shown in figure 2.9.
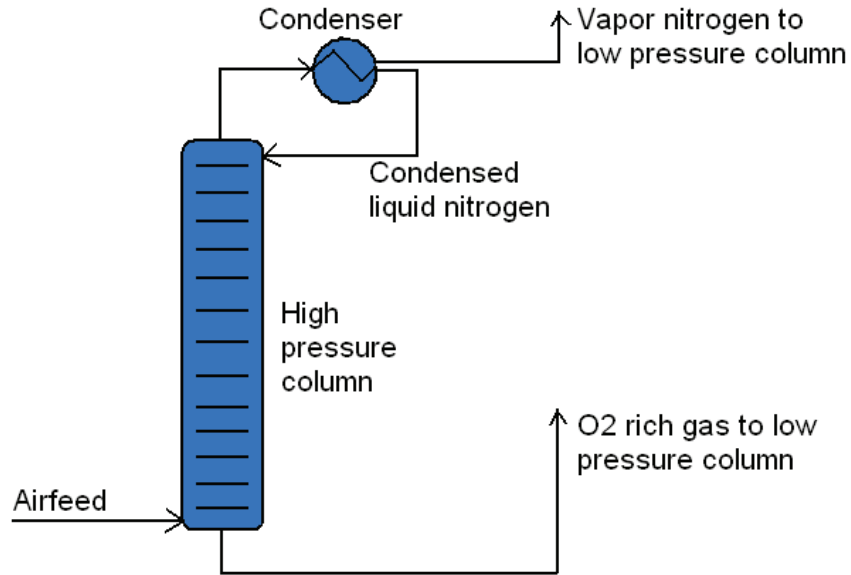
Figure 2.9. High pressure column.

The condenser in the column makes it possible to have a vapor nitrogen stream at a specified purity level. The condenser regenerates the top product to contain a certain amount of nitrogen. This may either be specified as a minimum nitrogen level or a maximum oxygen level. Typical nitrogen purity out of an air separation unit designed for IGCC is 99 percent and this is specified here [7]. There are two streams out of the condenser. They are separated by phase and the liquid phase stream is regenerated back to the top tray of the column while the vapor phase is sent to the LP column.

The O_2 rich gas from the bottom of the column can not be specified to contain a certain amount of oxygen, but varies with number of trays, pressure and temperature level and the purification level of the nitrogen stream in the top.

The number of trays in the column is an economic decision. More trays gives higher separation for lower condenser energy input, while less trays demands a higher rate of regeneration to achieve the specified nitrogen purity level.

2.1.2.6   Low pressure column

The low pressure column has three feed streams. The nitrogen stream from the high pressure column is fed to the top tray of the column. The O_2 rich stream from the high pressure column and the small air stream from the main heat exchanger are both fed about in the middle of the column. They are not necessarily fed to the same tray and what tray they exactly are fed to depend among other on the composition and temperature of the feed and the wanted outcome of the column. An overview of the low pressure column is shown in figure 2.10.
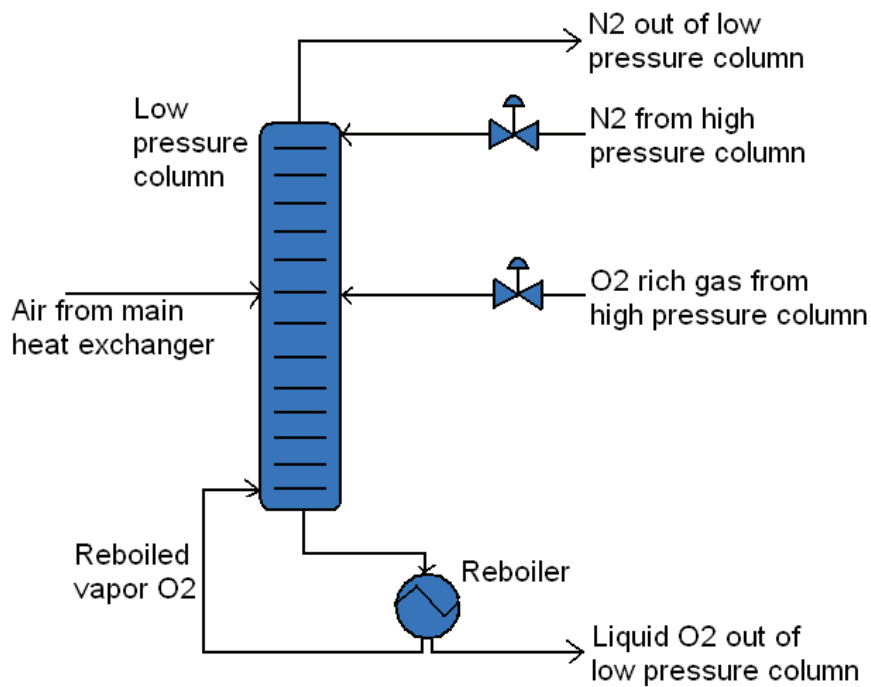
2.10. Low pressure column.

Both the nitrogen and the oxygen rich gas from the high pressure column are choked to a pressure level adjusted to the pressure at the feed tray. The relative pure nitrogen fed to the top tray is mixed with nitrogen from the column and taken out in the top of the column. This stream has nitrogen purity about the same level as the nitrogen purity specified from the high pressure column.

Instead of a condenser, the low pressure column contains a reboiler. The reboiler gives the opportunity to specify the oxygen purity in the outcome of the column. Out of the reboiler a vapor oxygen stream is regenerated into the bottom tray of the column while a liquid oxygen stream is sent out of the column. Typical oxygen purity needed for gasification purpose is 95 percent [11].

An analysis on number of trays is done similar to the analysis for the high pressure column.

2.1.2.7 Combined condenser and reboiler

A condenser needs cooling to condensate a gas while a reboiler needs heat to boil gas. It is possible to integrate the condenser in the high pressure column with the reboiler in the low pressure column. If this is done perfectly neither the condenser nor the reboiler need external duty to operate. The heat transferred away from the condenser is used to boil the oxygen in the reboiler. This process is shown in figure 2.11.
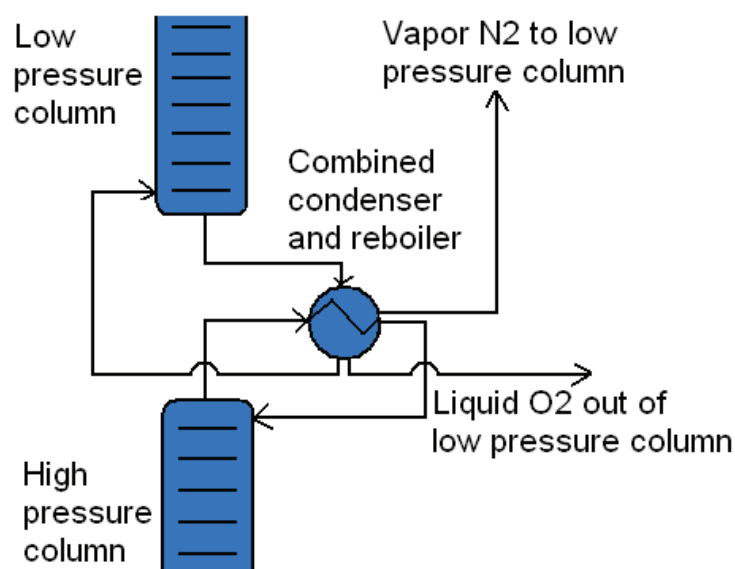
2.11. Combined condenser and reboiler.

The combined condenser and reboiler (CCR) is in other words an integrated heat exchanger. The temperature difference between the hot nitrogen stream and the cold oxygen stream has to be in accordance with the chosen ΔT.

As mentioned in *2.1.2.4 Main heat exchanger* a small amount of air is led out of the heat exchanger, expanded or choked and fed directly to the low pressure column. This is done mainly to get optimal mass flow and temperature differences through the combined condenser and reboiler. The amount of air fed directly to the low pressure column may vary, but is typically 10 percent [7].

2.1.2.8   Subcooler

The nitrogen rich stream between the high pressure and low pressure column needs to be cooled to a proper temperature level. This level is dependent on many factors as number of trays in the columns and the duty of the combined condenser and reboiler. To cool the nitrogen stream, the cold oxygen and nitrogen leaving respectively the bottom and the top of the low pressure column are utilized. This can be seen in figure 2.7.

2.1.2.9   After treatment of nitrogen and oxygen

The air separation island described delivers gaseous oxygen and nitrogen at a pressure level slightly above atmospheric pressure. Typical pressures are 1.5 to 2 bar [11]. The gases are as mentioned used to cool the incoming air and are therefore heated to about ambient temperature.

In an IGCC plant both the oxygen and nitrogen are utilized. The oxygen is used in the gasification process and the nitrogen is used to dilute the H_2 rich fuel before the gas turbine. The gasification pressure is ranging from 20 to 70 bar and even higher for modern gasifiers [6]. The gas turbine has a pressure level ranging from 10 to 35 depending on technology and size of the plant [16]. Oxygen and nitrogen both have to be compressed to fulfill their purpose in the IGCC plant. An overview of a complete air separation island including oxygen and nitrogen compression is shown in figure 2.12.
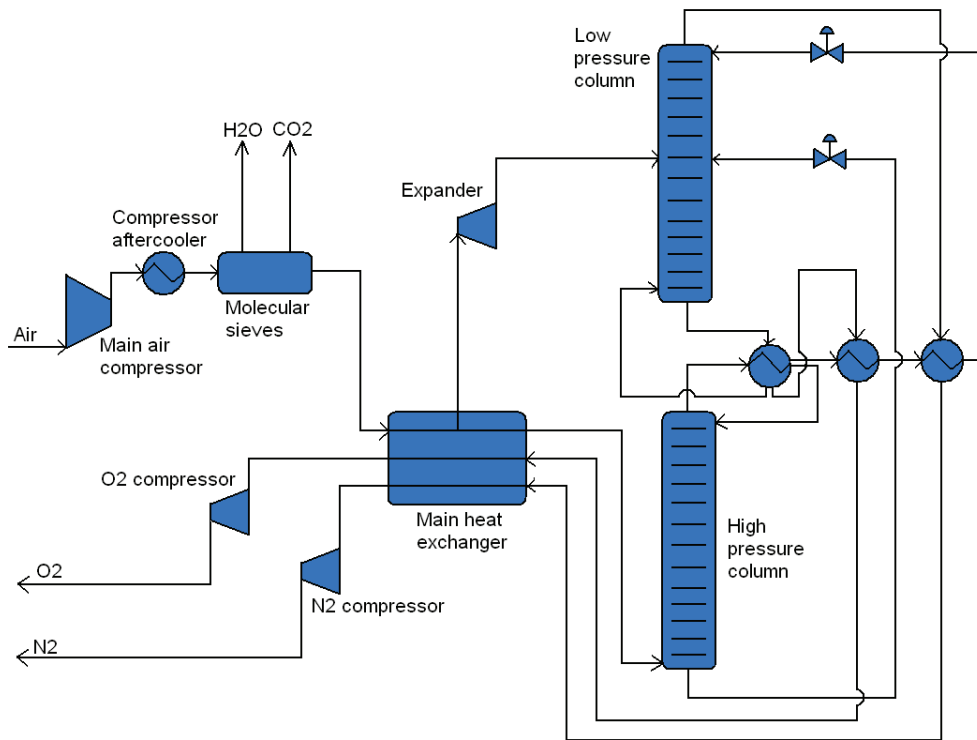
2.12. Air separation unit with after treatment.

As mentioned in *2.1.2.1 Introduction* is the energy cost of oxygen production 0.22 to 0.25 kWh per kg pure oxygen. In this energy analysis the after treatment is not included. This is because the compression rate varies with the use of the oxygen and the technology in subsequent processes. If compression after the main heat exchanger was included, different air separation units would be incomparable.

2.1.2.10 Liquid oxygen

The plant explained in the previous sections is a gaseous oxygen (GOX) production plant. It is also possible to produce oxygen in a liquid oxygen (LOX) plant. If the after treatment in the GOX plant is included, the outcome from a GOX and LOX plant is the same. The main difference is at what point in the plant the oxygen is compressed. Figure 2.13 gives an overview of a LOX plant.
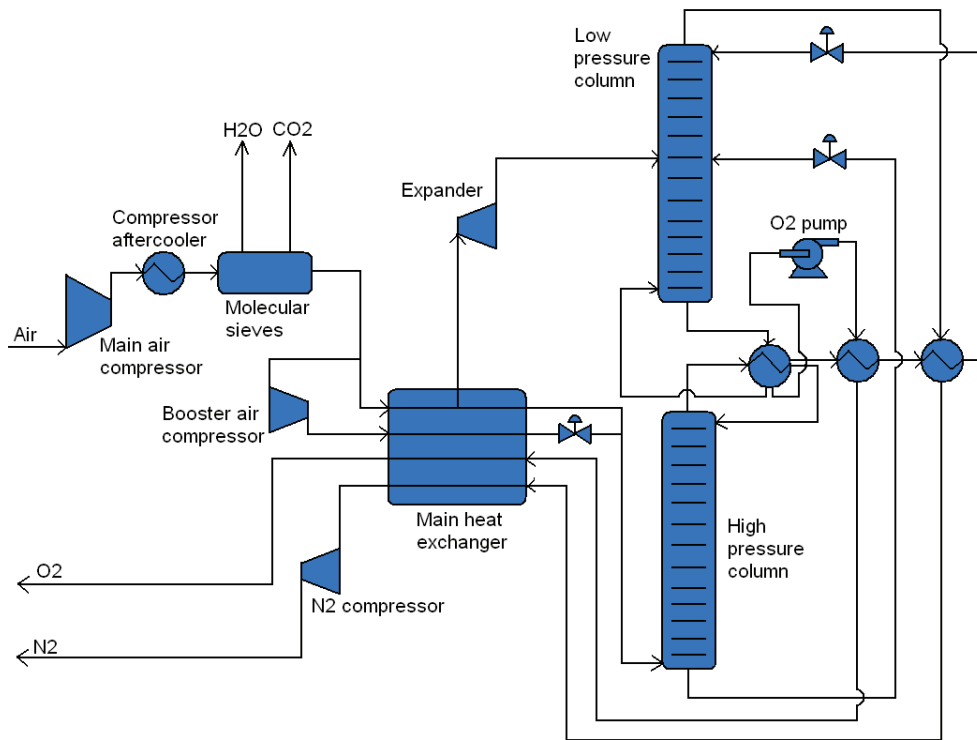
2.13. Liquid oxygen plant.

The main difference between GOX and LOX plants is as mentioned where the compression is done. The oxygen compressor after the main heat exchanger is replaced by an oxygen pump after the low pressure column. At this place the oxygen is in liquid phase and can easily be compressed to the wanted pressure. Pumping in liquid phase requires a remarkable lower energy demand than compression of gaseous oxygen. When oxygen is sent through the heat exchangers at high pressure and in liquid phase, it is not able to hand over as much cooling as the low pressure liquid oxygen in the GOX plant. In the GOX plant cooling energy due to phase transition is released in the heat exchanger before the main exchanger. In a LOX plant the phase transition cooling energy release is removed to main heat exchanger and there is need for external cooling of the nitrogen stream from the high pressure column.

Instead of external cooling the required coldness is produced internal. After the molecular sieves the air is split in two streams. The main stream is sent through the main heat exchanger as in a GOX unit. A smaller stream is further compressed and then cooled by air or water to ambient temperature before entering the main heat exchanger. This is done to remove more heat from the process when this air stream is choked back to high pressure column pressure. By doing this the air separation island again have no external cooling demand and the compression work is the only energy supplied the island. The amount of air through the

booster compressor varies with the additional coldness requirement, which again varies with wanted outcome pressure. The amount is typical 30 percent of the air feed [7].

There is an energy gain from having liquid oxygen pumped to wanted pressure instead of gaseous oxygen compressed. Almost all the energy gained is lost in the booster air compressor, but it is possible to reduce the total energy cost with 1 to 2 percent [7]. This percentage number is dependent on technology and the pressure level the oxygen out of the island is delivered at. Another advantage with LOX plants is the reduced explosion risk. There are always some risks when pure oxygen is compressed in gaseous form in a compressor. The risks are reduced when the pressure rise is done in liquid phase by a pump.

2.1.2.11   Argon treatment

In both the GOX and LOX plants described there is no capture of argon. Argon has its boiling point very close to oxygen and the separation process is thereby more complex [13]. Including argon separation demands an extra distillation column and due to the nearby boiling points between argon and oxygen, the column is a physical large construction. For IGCC purpose the traces of argon in both the oxygen and nitrogen streams are unimportant.

Argon has no utility value in an IGCC plant, but is used in other processes. It may therefore be an idea to include argon separation if other industries are willing to buy it. To decide whether an argon column should be included, an economic analysis concerning the price of argon compared to the price of an extra column plus the extra energy demand must be discussed. An air separation island including argon treatment is shown in figure 2.14.
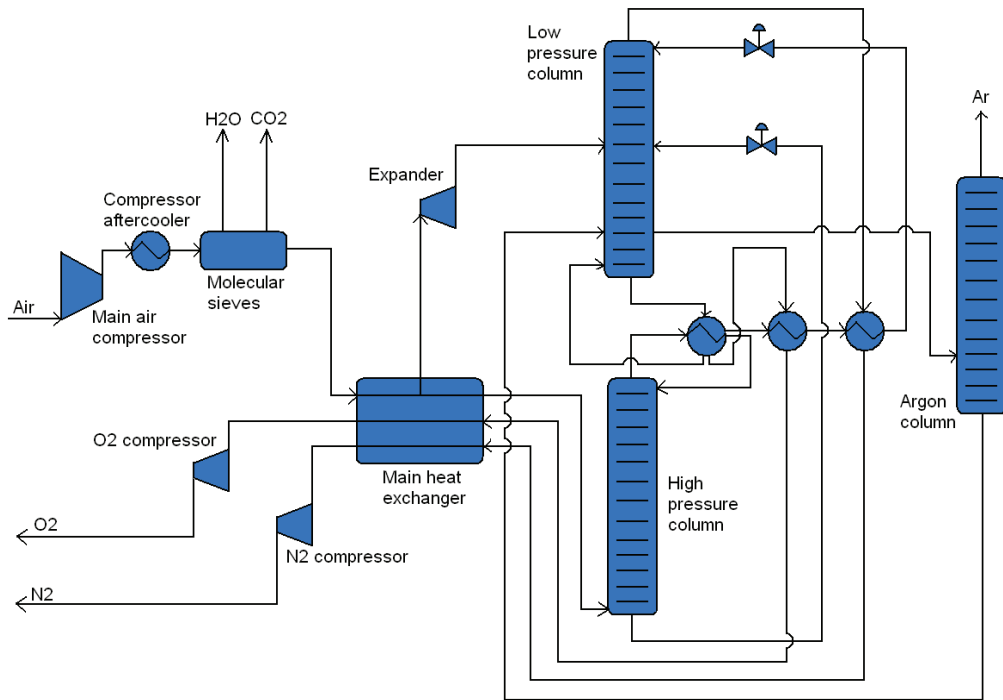
Figure 2.14. GOX plant with argon treatment.

At a tray in the lower part of the low pressure column the entire flow going through the column is taken out and sent to the argon column. The flow is fed to the argon column near the bottom. In the argon column argon is separated from the oxygen rich feed and sent out as top product. The bottom product now contains only small traces of argon and is sent back to the low pressure column. The feed tray of the bottom product is directly under the tray where the flow was taken out and sent to the argon column.

2.2   Gasification Island

2.2.1   Coal

Coal is the most common source for electricity production all around the world. Coal provides 25% of global primary energy needs and generates 40% of the world's electricity [17].The consumption of coal is still increasing, especially in China, and it is expected that it will play a major role as an energy source the next decades. The remaining resources of coal around the world is proved to be significant larger than for oil and gas. The ratio of reserves to current production (R/P ratio) is 147, which means that with today's coal consumption the world's reserves will last 147 years. Corresponding numbers for oil and gas are respectively 40 and 63 [5]. These numbers varies from different sources. *Gasification* estimates with an R/P ratio for coal as 216 [6]. Anyhow this demonstrates that coal will be an important part of the energy market in the upcoming years.

Coal fired power plants are one of the largest source of CO_2 world wide. A reduction of coal consumption in the nearest future seems unrealistic. CO_2 capture from coal fired power plants will probably become one of the main sources to reduce CO_2 emissions.

One of the actual technologies of CO_2 capture from coal fired power plants is to gasify the coal and thereafter extract the CO_2 before the power cycle. This gasifying process will be studied closer in the following chapters.

2.2.1.1   Composition

The composition of coal is complex. The resources are distributed all over the world and the formation process of coal differs and depends on location. Because of the variations in properties it is hard to make one definition of coal. The varying compositions cause different properties which affect the performance for instance in a power plant. The main components in coals are carbon, hydrogen, oxygen, nitrogen and sulfur. The amount of the different substances decides the heating value of the fuel. Table 2.3 shows the composition and lower heating value of several types of coal from different regions in the world.

Table 2.3. Variation of coal composition [6].

Coal		Composition					LHV
Country, region	Class	C	H	O	N	S	MJ/kg
Germany, Ruhr	Anthracite	91.8	3.6	2.5	1.4	0.7	36.2
Australia, typical	Bituminous	81.3	5.8	10.0	2.0	0.9	33.8
India, typical	Bituminous	75.5	6.4	15.2	1.5	1.4	32.1
China, Datung	Bituminous	84.4	4.4	9.5	0.9	0.8	33.4
South Africa, typical	Bituminous	83.8	4.8	8.4	2.0	1.0	34.0
Poland, typical	Bituminous	82.8	5.1	10.1	1.4	0.6	36.1
USA, Illinois	Bituminous	78.4	5.4	9.9	1.4	4.9	33.7
USA, Montana	Sub-bitiminous	76.4	5.6	14.9	1.7	1.4	31.8
USA, North Dakota	Lignite/browncoal	71.0	4.3	23.2	1.1	0.4	26.7
Germany, Rhein	Lignite/browncoal	67.5	5.0	26.5	0.5	0.5	26.2

The composition data of coal can be presented in different ways. There are four classifications for coal description [12]. Those are as-received (ar), moisture-free (mf), ash-free (af) and ash-and-moisture-free (maf) basis. Table 2.3 shows the composition on a maf basis. That means that the moist and ash is not included in the composition and heating value calculations.

2.2.1.2   Proximate analysis

This analysis method helps to determine the composition on a macro level. That means to decide the fractions of moisture, volatile matter, ash and fixed carbon. Moisture is found both on the surface and inside the coal particles. The amount of moisture can vary from a few percent to 60-70% dependent on the coal type. The moisture is determined by drying the coal for 1 hour under standard coal drying conditions at 104-110˚C. [6] Volatile matter is a mixture of many components. The most common are hydrocarbon gases, lighter oil, tar, hydrogen and water. To determine the volatile matter the coal is heated for 7 minutes to about 950˚C. The rest, which now can be completely combusted, is the fixed carbon. The amount of fixed carbon can be determined by measure the mass loss. When coal is classified it is ranked after the fraction of fixed carbon. Table 2.4 shows the numerical values for the most common coal classifications. Anthracite has the highest fixed carbon value and therefore the highest heating value. Anthracite is thus classified as a high ranked coal while Lignite is in the category of low ranked coal.

Table 2.4. Classification of coal [6].

Classification of coal			
Class	**Volatile matter**	**Fixed carbon**	**Heating value**
	wt%	wt%	MJ/kg
Anthracite	<8	>92	36-37
Bituminous	8-22	78-92	32-36
Sub-bituminous	22-27	73-78	28-32
Lignite/browncoal	27-35	65-73	26-28

2.2.1.3 Ultimate analysis

The ultimate analysis gives the percentages of the elements in coal, mainly carbon, hydrogen, oxygen, nitrogen and sulfur. Table 2.3 shows a typical ultimate analysis of different coals on mass basis. The browncoal from Rhein, Germany, contains for example 67.5% carbon on mass basis.

There are also traces of a lot of other minerals in coal. Actually a substantially part of the periodic table can be shown to be present in coals [6]. For the case of simplicity these components will be neglected in the calculation in this report. Despite their relatively low fractions, they will play a role connected to gasification and power production. A typical issue is damage on machinery which requires removal of some of the substances.

2.2.1.4 Conversion to gas

The process of converting coal to a useable gas is complex and passes different stages. The main stages are drying, pyrolysis and gasification. In a normal combustion process the combustible matter goes through these three stages before the final combustion which releases heat. In this case, the issue is to get the intermediate matter between gasification and final combustion and use that gas in a gas turbine. This is called synthetic gas or just syngas and it is mainly a mixture of carbon monoxide (CO) and hydrogen (H_2).
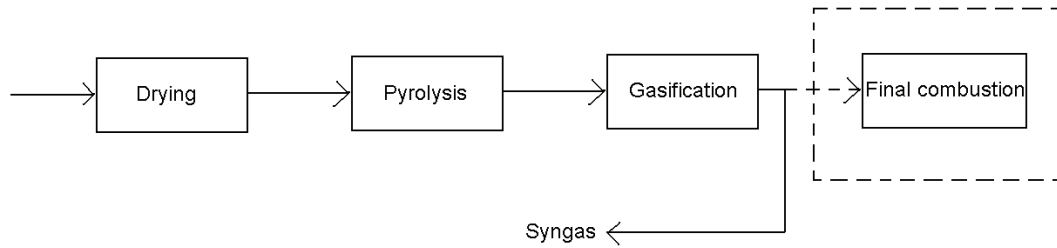
Figure 2.15. Transforming coal to syngas.

Before the final gasification stage the coal goes through the drying and the pyrolysis processes. There will be given a short explanation of these stages before the final gasification is discussed in detail.

In theory, the stages appear chronological corresponding to Figure 2.15. One stage does not start until the previous stage is completely finished. In practice there is not a total separation of the stages and they are overlapped by each other. Figure 2.15 shows an overview of the different stages in a coal conversion process. In the modeling work presented later the whole conversion process will occur in one unit and the operation is described only as gasification. In fact there will also be implemented a shift reactor to maximize hydrogen production as well.

Drying and pyrolysis

The drying and pyrolysis are not separate units, but are included as steps in the gasification in the gasifier. Combustion of coal requires dry coal. A gasifier can use additional steam supply and/or the humidity in the coal can operate as a reactant in the gasification reaction [10].

Drying is the easiest part of the process. The principle is simply to heat up the coal particles. Even though drying is not technological advanced the speed of the heating has influence on the next steps. With a slow temperature rise the subsequent steps are more or less separated. A fast rise in temperature leads to pyrolysis and gasification in one simultaneous process. This is shown in Figure 2.16.
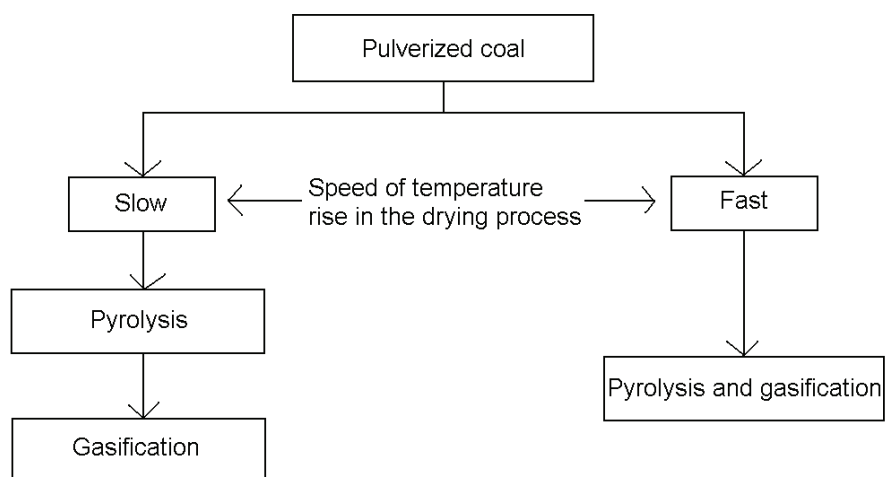
Figure 2.16: Influence of heating rate [17].

Pyrolysis of coal is also known as *devolatilization* or *carbonization*. It refers to the decomposition of organic matter by heat in the absence of air [18].The hydrogen rich volatile matter is removed and a carbon-rich solid part is left behind. From pyrolysis one can go further and produce liquid or gasses. Anyway pyrolysis is considered as the first conversion step in the process. The pyrolysis products depend on the raw material. For coal the composition is complicated and varying. Coal contains an inhomogeneous mixture of different organic and inorganic materials which varies from type to type. The complex composition of coal makes the pyrolysis hard to describe. There will always be an approximation instead of an exact answer in determining the pyrolysis process [18].

The knowledge concerning the pyrolysis process is not fully developed and further details will not be discussed in this report. The gasification process will be study in details in the next part.

2.2.2   Gasification

Gasification occurs when the fuel reacts with steam and oxygen under given conditions. In this case the fuel is consider as coal containing carbon, hydrogen, nitrogen, oxygen and sulfur. Some gasification processes use air instead of oxygen. In this report air gasification is left out. With air the fraction of inert N_2 is high and it will require larger equipment to reach the same production rate as an O_2 gasifier.
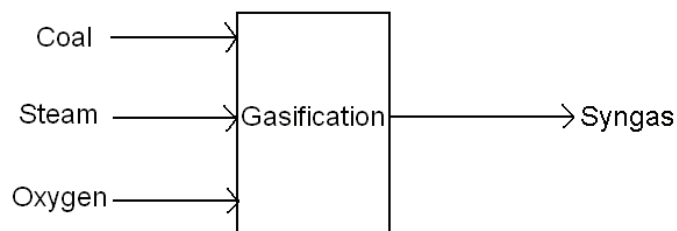
Figure 2.17. Gasification process.

Figure 2.17 gives an overview of what occurs in the gasification process. Coal reacts with steam and oxygen and creates syngas. Syngas is a mixture of carbon monoxide and hydrogen. In addition to CO and H_2 the reactions will form other products that will be described through this section, but the goal is to optimize CO and H_2 production since these can be utilized in a gas turbine. For coals containing moisture there may be unnecessary to add steam.

The gasification process can be represented by equilibrium conditions and to describe gasification it is possible to set up an innumerable number of reactions between carbon, hydrogen, oxygen, water, nitrogen and sulfur.

2.2.2.1   Formation reactions

The first step to calculate the output composition from the gasifier is to look at the formation reactions [18].

$$C + 1/2\,O_2 \rightleftharpoons CO \qquad\qquad\qquad -111\text{MJ/kmol} \qquad\qquad (2.30)$$

$$C + O_2 \rightarrow CO_2 \qquad\qquad\qquad -394\text{MJ/kmol} \qquad\qquad (2.31)$$
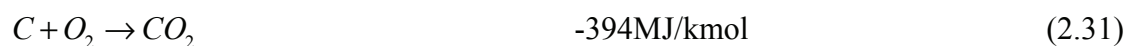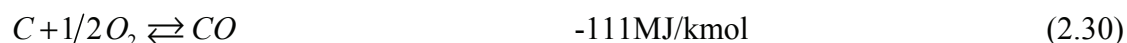
Equation 2.30 and 2.31 shows the *oxygenolysis* where carbon reacts with oxygen to form carbon monoxide and/or carbon dioxide. In this case the oxygen feed will occur as pure oxygen and not in an air mixture. Equation 2.31 is the combustion reaction for pure carbon. Sufficient amount of O_2 gives complete combustion and creates CO_2. For gasification the CO formation step is important. This occurs when there is deficiency of O_2 in a high temperature

reactor, above 800˚C [18].The corresponding heat of reaction states if the reactions are endothermic or exothermic. A negative sign indicates an exothermic reaction meaning that the reaction will liberate energy, and opposite for a positive sign. The values of the heat of the reaction are temperature dependent and are here determined for 25˚C (298K). The variation of the value will though not vary significantly with temperature, as an example the value for equation 2.30 will increase approximately 5MJ/kmol if the temperature is increased to 1500K.

With deficit of oxygen C may react with CO_2 according to the Boudouard reaction [18].

$$C + CO_2 \rightleftarrows 2CO \qquad\qquad +172\text{MJ/kmol} \qquad\qquad (2.32)$$
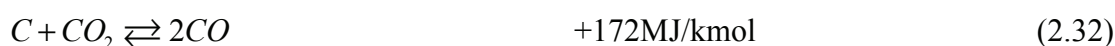
Methane will also be formed when carbon reacts with hydrogen. This reaction is called *hydrogenolysis*. The hydrogen comes from the coal and from the water feed. The later explained *hydrolysis* reaction contributes to produce pure H_2 [18].

$$C + 2H_2 \rightleftarrows CH_4 \qquad\qquad -75\text{MJ/kmol} \qquad\qquad (2.33)$$
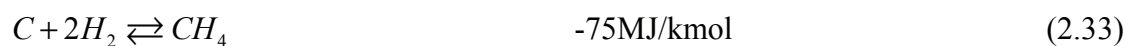
Reaction 2.30 and 2.33 react inverse according to temperature. The production of CO increases with increasing temperature while the CH_4 production is on a maximum level around 300˚C and decreases with increasing temperature. For power applications with CO_2 capture the formation of CO is of interests and reaction 2.30 plays the major role compared to reaction 2.33. The formation of CO is important because it can react with H_2O in a water gas shift reaction and create H_2. This reaction will be discussed in *2.2.2.4 Water gas shift reaction*.

Converting coal to syngas involves water, fed as steam or as a part of the coal. Reaction with water is called *hydrolysis* or *water gas reaction* and it is an endothermic reaction [18].

$$C + H_2O \rightleftarrows CO + H_2 \qquad\qquad +131\text{MJ/kmol} \qquad\qquad (2.34)$$

The water gas reaction also produces more syngas with higher temperature. The partial pressure of water steam is proportional with syngas production as well.

Equation 2.30 and 2.34 describe the most relevant gasification reactions for this case. The heats of reactions show that reaction 2.30 is exothermic and reaction 2.34 is endothermic. That indicates that most of the gasification will occur via reaction 2.30. On the other hand there will be more economical to maximize reaction 2.34. This reaction yields two syngas molecules per atom of carbon, while the first reaction only gives one syngas molecule. Another issue is that steam is cheaper than oxygen, so one in this case one will anyway gain on maximizing the water gas reaction.

Formation of water as a result of hydrogen combustion appears in a well known equation [18].

$$H_2 + 1/2\,O_2 \rightleftarrows H_2O \qquad\qquad \text{-242MJ/kmol} \qquad\qquad (2.35)$$
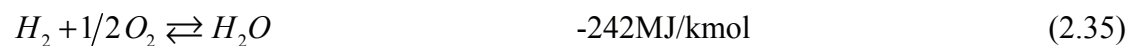
The nitrogen and sulfur will react with the oxygen and form equilibrium with nitric oxide (NO) and sulfur oxide (SO_2) [18].

$$1/2\,N_2 + 1/2\,O_2 \rightleftarrows NO \qquad\qquad \text{+90MJ/kmol} \qquad\qquad (2.36)$$

$$S + O_2 \rightleftarrows SO_2 \qquad\qquad \text{-362MJ/kmol} \qquad\qquad (2.37)$$
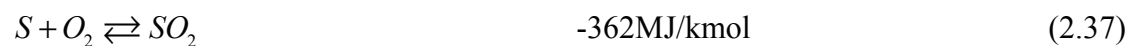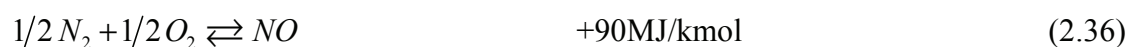
These substances are represented in small amounts, but they play an important role in the pollution calculation and they are therefore not neglected.

The sulfur will in a gasification process also react with the hydrogen and create the acid gas hydrogen sulfide (H_2S) [18].

$$S + H_2 \rightleftarrows H_2S \qquad\qquad \text{-85MJ/kmol} \qquad\qquad (2.38)$$
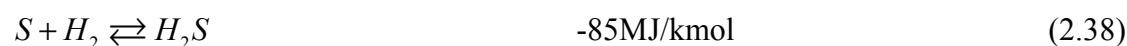
The gasification process occurs as a set of exothermic and endothermic reactions. There will in a gasification process be an increasing in temperature during the process. This indicates that some of the chemical energy is transformed to heat. The amount of chemical energy in the product gas compared to the amount of energy in the feedstock can be expressed as the cold gas efficiency (CGE).

$$CGE = \frac{LHV_{product}}{LHV_{feedstock}} \qquad (2.39)$$

Normal value for CGE is around 0.8 or 80 % [6].

2.2.2.2 Equilibrium equations

The gasification process will roughly appear under equilibrium conditions. Equilibrium states are helpful for deciding the composition of substances after the gasification. Equation 2.30, 2.31, 2.33, 2.35, 2.36, 2.37 and 2.38 can be rearranged at equilibrium form [18] [19].

$$K_{CO} = \frac{\left[y_{CO}\right]}{\left[y_C\right]\left[y_{O_2}\right]^{\frac{1}{2}} p^{\frac{1}{2}}} \qquad (2.40)$$

$$K_{CO_2} = \frac{\left[y_{CO_2}\right]}{\left[y_C\right]\left[y_{O_2}\right] p} \qquad (2.41)$$

$$K_{H_2O} = \frac{\left[y_{H_2O}\right]}{\left[y_{H_2}\right]\left[y_{O_2}\right] p^{\frac{1}{2}}} \qquad (2.42)$$

$$K_{CH_4} = \frac{\left[y_{CH_4}\right]}{\left[y_C\right]\left[y_{H_2}\right]^2 p^2} \qquad (2.43)$$

$$K_{NO} = \frac{\left[y_{NO}\right]}{\left[y_{O_2}\right]^{\frac{1}{2}}\left[y_{N_2}\right]^{\frac{1}{2}}} \qquad (2.44)$$

$$K_{SO_2} = \frac{\left[y_{SO_2}\right]}{\left[y_S\right]\left[y_{O_2}\right] p} \qquad (2.45)$$

$$K_{H_2S} = \frac{\left[y_{H_2S}\right]}{\left[y_S\right]\left[y_{H_2}\right] p} \qquad (2.46)$$

For the equilibrium equations K_i is the equilibrium constant, y_i indicates the molar fraction of the substances and p the pressure. In fact K_i is not constant but temperature dependent. The values of K_i for a given temperature are tabulated. In a gasification system the temperature will vary a lot during the process and the equilibrium "constant" has to be modeled as a function of the temperature.

In a reactor producing syngas a lot of reactions occur at the same time. Substances will be created and broken during the process. Equation 2.30 to 2.38 shows the main reactions in converting coal, oxygen and steam into synthetic gas. The most interesting component in coal is the carbon. It is the main energy carrier and its heating value is of interests for the power production. In fact hydrogen has a higher heating value than carbon on mass basis, but there is normally significant less amount of it in the coal.

The main product of a gasification process is carbon monoxide and hydrogen. A typical molar product composition is about 60% CO, 30% H_2 and the remaining 10% consist mainly of CO_2, H_2O, CH_4, NO_x, SO_x and H_2S. The amount of these substances will vary according to coal type, gasification conditions (temperature and pressure) and the amount of oxygen and steam in the feed.

The gasification process will be described in more details in *2.2.3 Gasification procedures*. First there will be given short explanation about syngas and the water gas shift reaction.

2.2.2.3 Syngas

Syngas is shorthand for synthesis gas and consist of CO and H_2. Other substances in the product of a gasification process are H_2O, CO_2 and CH_4 etc. The composition is reliant of both pressure and temperature in the gasifier. For increasing pressure the amount of CO and H_2 are decreasing and the other substances increases correspondingly. For increasing temperature the amount of CO rise and the amount of H_2O, CO_2 and CH_4 decreases to compensate for the increase in CO. The H_2 quantity is almost constant through temperature oscillations [6].

Syngas is used in a lot of chemical manufacturing processes, for example the production of ammonia and methanol. In this report the application is focused on power production. Syngas itself can be utilized in a power cycle using the same principles as a conventional gas turbine. Syngas can also be converted to a hydrogen rich gas before it enters a power cycle. The reason for this is to increase the partial pressure of CO_2 which makes it easier to remove it. To manage this, a water gas shift reactor can be installed.

2.2.2.4 Water gas shift reaction

For a power plant without CO_2 capture the gasification products CO and H_2 is suitable for a gas turbine. For a power plant with CO_2 capture the final target in the coal conversion is to maximize the hydrogen production. This will occur according to the water shift reaction [18].

$$CO + H_2O \rightleftarrows CO_2 + H_2 \qquad\qquad \text{-41MJ/kmol} \qquad\qquad (2.47)$$

An overview of the water shift is given in figure 2.18.
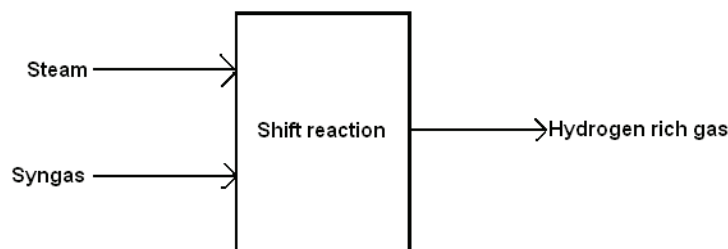
Figure 2.18. Input and output in a water gas shift reactor.

Carbon monoxide transfers its heating value to the hydrogen through a reaction with water steam. H_2 has a molar lower heating value of 241.8MJ/kmol and CO has a corresponding value of 283.0MJ/kmol [20]. This different is released as heat, and it agrees with the number from equation 2.47. This indicates that some of the chemical energy generates heat and therefore gives a heat loss, exothermic reaction. A typical operation temperature of a shift reactor is between 200˚C and 500˚C [20]. Some of this heat may be regained and utilized in other processes in a power plant.

The carbon binds up to the oxygen and creates non combustible carbon dioxide. A typical CO conversion factor is about 0.98 which means that 98% of the CO will convert to CO_2 [10]. The product composition of a shift reactor is characterized with high hydrogen content, typical value of 50%. The CO_2 fraction lies in the area around 30-40% and the remaining substance is small amount of H_2O, CO, CH_4, H_2S, SO2**,** N_2 and NO_X.

The temperature in a shift reactor is relatively low compared to the gasification reactor. A typical shift reformer temperature lies in the area between 200˚C and 500˚C [20]. For this low temperature the exothermic reaction will turn to the right and favor hydrogen production. To

maximize the production of H_2, the water shift often occurs in two stages with a cooler between the stages. The temperature from the gasifier can be as high as 1600˚C and a heat exchanger is required also here to move away heat before the shift reaction [20]. In a combined cycle this heat can be implemented in the steam cycle to improve efficiency. In a plant like this were the shift reactor comes after a gasification reactor the pressure will remain the same in both reactors except the pressure loss.

Particles and acid gases as SO_2 and H_2S have to be removed before the power cycle. CO_2 is also an acid gas that can be removed together with SO_2 and H_2S.

2.2.3   Gasification procedures

The gasification process will here be discussed more detailed. This is because the gasification process has more variables than the water shift. The gasification is very dependent on the feed, and for coal gasification this is varying for different coal types. The water shift reaction for H_2 production is not varying that much. The products from the gasifier are much the same since oxygen and steam is regulating the product stream into wanted composition. For power production this will be about 60% CO and 30% H_2 while the last 10% is mainly CO_2, N_2 H_2S etc [6].

The gasification process occurs as mention as a reaction between the feedstock, oxygen and/or water steam. It is clear that the amount of the different reactants affect the product. In addition pressure and temperature also play a role in the gasification. The gasification rate can be measured as a carbon conversion rate. That means the fraction of carbon that is gasified to the fraction of carbon in the feedstock [6].

$$C_{conversion} = \frac{C_{product}\left[kmol\right]}{C_{feedstock}\left[kmol\right]} \qquad\qquad (2.48)$$

The conversion rate lies closed to 1 (100%) for modern gasification reactors.

One can assume the coal feed as a given composition. There will off course appear different coal types in a gasifier, but for each coal type a modeling/calculation can be done. The coal feed is given and the gasification process is regulated by the amount of feed, steam and

oxygen. 1mol of coal will normally consume from 0.2 to 0.5mol oxygen. The amount of steam and oxygen regulates the temperature and the wanted composition. The general rule is that CO production is favored with stoichiometric deficiency of O_2 at high temperature (1500˚C). It is obvious that the hydrogen production will increase with increasing steam rates, but it is a limit how much of the water that is converted. For optimization the H_2 production rate, the mentioned shift reactor is installed.

Temperature plays a major role in gasification when it directly affects the composition of the product. At low temperatures production of methane is favored, while higher temperature increases the syngas ($CO + H_2$) production. Modern gasifiers, which are designed for syngas production, operate at temperature levels up to 1500˚C and even higher [6]. Increasing the amount of O_2 in the gasifier increases the temperature while injection of water steam works opposite.

The pressure will not affect the compositions considerably. There are however advantages to gasify under pressure regarding to equipment size and compression energy. Modern processes are operated at pressures from 10bar and up to 100bar [6]. For an IGCC application the normal operating pressure lays in the area between 15bar and 40bar [16]. When CO_2 capture is implemented a high pressure is required to ease the capture procedure [10].

There are different gasification reactors. The reactor type strongly influence the temperature distribution, and in this way the product composition [18]. The main gasification procedures are *moving-bed gasifiers, fluid-bed gasifiers* and *entrained flow gasifiers.* The last one is most relevant for IGCC applications. In the upcoming chapters the moving-bed and the fluidized bed methods will be discussed briefly, before the entrained flow gasification system will be discussed closer.

2.2.3.1　　Moving-bed gasifiers

Moving-bed is the oldest gasification process and it played an important role of producing syngas from coal in the early stages of gasification. This technology is often called fixed-bed gasifier. The principle of this process is that the gravity drags the feedstock (here coal) slowly downwards and the gasification occur when a counter-current blast reacts with the coal. The gasification products (syngas) flow upwards and preheat the down flowing coal. An overview

of this process is given in figure 2.19. Moving-bed process is characterized with low oxygen consumption and a relatively low outlet temperature. A negative factor of this process is that the low temperature and the low oxygen consumption affect the gasification rate. Not all of the feed is gasified and there are pyrolysis products presented in the syngas. Moving-bed gasifiers have moving parts like for example a stirrer. These equipments required a relatively high amount of maintenance [6].
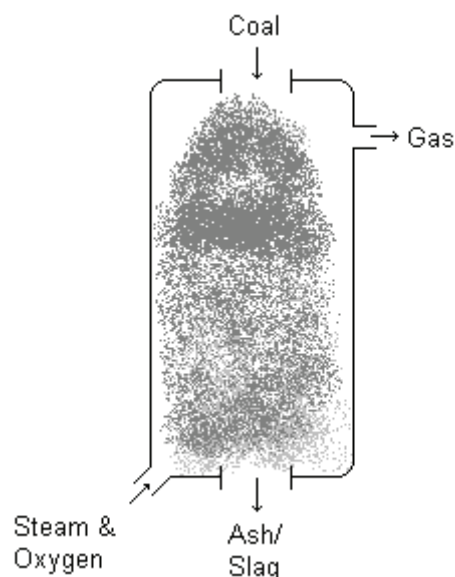
Figure 2.19. Lurgi Dry Ash Gasifier.

A very common moving-bed patent is the Lurgi Dry Ash Gasifier. The principles here are the same as for a general moving-bed facility. The Lurgi process is however using pure O_2 in the gasification process instead of air and it operates under higher pressure than atmospheric. Pulverized coal is fed from the top via a lock hopper. The lock hopper technology will be discussed closer in chapter *2.2.3.5 Feeding procedures for a gasifier*. The coal is spread in the reactor by a mechanical distribution device and moves slowly downwards undergoing the gasification process reacting with O_2 and water steam. The Lurgi reactor vessel is a double-walled room where the space between the walls is filled with boiling water. This is used as cooling as well as reactant in the gasification process [6].

The composition of the product gas from a Lurgi gasifier depends on the composition of the feedstock. For coal gasification this means the ranking of the coal according to carbon content, hydrogen content etc. A rough estimate of the product gases from this type of a gasifier gives around 30% CO_2, 20% CO and 40% H_2 on molar basis. The last 10% is a

mixture of CH_4, N_2 and other trace elements. These numbers varies though according to coal type, but it gives a useable overview. Carbon conversion rate can be as high as 99% [6].

Lurgi gasifiers are spread all over the world. The SASOL complex in South Africa is the largest gasification plant in the world according to Higmans Gasification edition from 2003. This plant uses Lurgi dry ash gasifiers and produces 55million Nm^3 per day.

Other commercial Moving-bed gasifiers are British Gas/Lurgi (BGL) Slagging Gasifier and the Ruhr 100 gasifier. The BGL is an improvement of the Lurgi gasifiers designed for slagging conditions. This gives an increasing in CO production and a reduction in the steam consumption. The Ruhr 100 gasifier is a version of the Lurgi gasifier constructed to handle high pressure, 100 bar[6].

2.2.3.2   Fluid-bed gasifiers

Fluidized bed gasifiers are fed with pulverized coal and this is lifted by feed and product gasses. Steam/oxygen is fed near bottom and mixes with the pulverized coal and reacts while the fluidized state is kept.

This technology gives a good mixing between feed and oxygen/air and steam. It operates at relatively low temperature as low as 800˚C for biomass and 950˚C for coal. For coal gasification the carbon conversion rate is low. The best of existing facilities have a rate up to 97%. Low ranked coal and biomass are more suitable for a fluid-bed gasifier. These are reactive feedstock which not requires too high temperature and the conversion rate may then exceed 99%. Problem with fluidizing coal is the case that coal differs so much in shape and composition. The particles should not be larger than 10 mm. However too small particles will entrain in the syngas and not get satisfactory gasified. A more detailed description will not be given here because for the purpose of IGCC plants, this technology is not relevant [6] [18].

2.2.3.3   Entrained-flow gasifiers

Entrained-flow gasifiers are the most common for using in IGCC plants. It operates under high temperature and requires considerable amounts of oxygen. The gasifier is very flexible according to feedstock and all coal types can be fed. However, coals with high moisture will

require more oxygen. For those coals alternative processes may be economical more beneficial. Entrained-flow gasifiers operate at pressures from 20 to 70bar and at a temperature of at least 1400˚C. The operation temperature is above the ash melting point which implies that these gasifiers are of the slagging type. As a result of that, tar and oils are destructed and the carbon conversion rate is high, over 99%. Another advantage with this process is the relatively low methane content in the product gas. This gives a better quality of the syngas. An entrained flow gasifier has a relatively low H_2/CO ratio. A shift reactor is required if higher H_2 fraction is wanted.

The reactor of an entrained-flow gasifier is characterized with a concurrently flow of feed, oxygen and steam. If the feed is so called coal-water slurry, the steam may be left out. This is because there is sufficient amount of water in the mixture already. Figure 2.20 shows a simple sketch of a gasifier for dry coal with the feed entrance at the top.
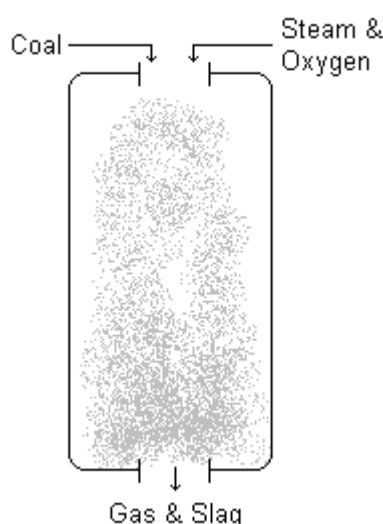
Figure 2.20. Top-Fired Dry Coal Feed Slagging Entrained-Flow Gasifier.

Since the coal is dry, water supply is required. The Top-Fired equipment differs from Side-Fired gasifiers according to where the coal and oxygen/steam is fed. In a Side-Fired installation coal, oxygen and steam are fed from one or two sides and the product gas flows up and the slag goes to the bottom.

As mentioned all coal types are usable in an entrained-flow gasifier. Coals with too much moisture are for economical reasons not attractive when too much energy is required to

evaporate the water. This yields first of all for browncoal/lignite. The same principle counts for the case of ash. Ash has to be melted and a high fraction of this also contributes to a higher duty for the gasifier.

Dry coal gasifiers need less oxygen than coal-water feed gasifiers, in practice the consumption is 20-25% lower. Production of oxygen is energy demanding and this value gives a considerable influence of the total energy consumption. Coal-water slurry feed has its advantages that it is easier to pressurize. The dry-feed installations require advanced lock hopper technology to reach satisfactory pressure, and the ultimate pressure for these facilities is about 50bar. The corresponding value for the coal-water slurry-feed-gasifiers can be as high as 200bar. This is a result of the fact that a mixture containing water than can be pressurized using a pump. This not a simple operation, but it is simpler than the lock hopper method [6].

Since coal differs in composition the behavior in the gasification process also differs a lot. Table 2.5 shows the product gas from different coal types in a typical Dry-Coal Entrained-Flow Gasifier.

Table 2.5. Coal performance in dry-coal entrained-flow gasifiers [6].

Performance of various types of coals in Dry-Coal Entrained-Flow Gasifiers								
Coal			**Mol Fraction Product Gas**					
Country	Region	Classification	CO	H_2	CO_2	N_2	A	H_2S
Germany	Rhein	Browncoal	0.61	0.29	0.08	0.01	0.01	0.002
USA	North Dakota	Lignite	0.62	0.26	0.1	0.01	0.01	0.001
USA	Montana	Sub-bituminous	0.63	0.34	0.01	0.01	0.01	0.004
USA	Illinois	Bituminous	0.61	0.35	0.01	0.01	0.01	0.015
Poland	typical	Bituminous	0.58	0.39	0.01	0.01	0.01	0.002
S.Africa	typical	Bituminous	0.64	0.33	0.01	0.01	0.01	0.003
China	Datung	Bituminous	0.66	0.31	0.01	0.01	0.01	0.002
India	typical	Bituminous	0.62	0.33	0.02	0.01	0.01	0.005
Australia	typical	Bituminous	0.62	0.34	0.01	0.01	0.01	0.003
Germany	Ruhr	Anthracite	0.65	0.31	0.01	0.01	0.01	0.002

From table 2.5 one can see that the syngas composition not differ too much from various coal types. Studying table 2.6 gives a better impression taken into account the oxygen consumption

and the production of wanted syngas compared to the amount of fuel. The German Anthracite gives more than twice the amount of syngas compared to the German Browncoal. There is however a high steam consumption in the conversion process containing Anthracite.

Table 2.6. Including oxygen consumption [6].

Coal			Amount of reactants and products		
Country	Region	Classification	Nm^3 syngas/ ton maf coal	Nm^3 O_2/ Nm^3 CO+H_2	kg steam/ Nm^3 CO+H_2
Germany	Rhein	Browncoal	965	0.33	0
USA	North Dakota	Lignite	935	0.36	0
USA	Montana	Sub-bituminous	1950	0.26	0.06
USA	Illinois	Bituminous	2030	0.25	0.09
Poland	Typical	Bituminous	2290	0.20	0.15
S.Africa	Typical	Bituminous	2070	0.26	0.09
China	Datung	Bituminous	2060	0.27	0.09
India	Typical	Bituminous	1730	0.31	0
Australia	Typical	Bituminous	2100	0.26	0.07
Germany	Ruhr	Anthracite	2270	0.26	0.13

Entrained flow gasifiers are the most common for IGCC application. An introduction to some of the commercial developed gasifiers of this type will be given below [6] [18].

2.2.3.4   Different entrained-flow gasification processes

The first commercial entrained-flow gasifier was the Koppers-Totzek (KT) process which was developed in the 1950s, and units were built several places around the world [6]. This process operated at atmospheric pressure and it will not be described in detail since improved versions are introduced. The newer facilities are based on the KT process but have improvements according to for example higher operating pressure. A modern KT-based entrained flow gasifier is the Shell Coal Gasification Process (SCGP). This process will be discussed closer in the upcoming part.

There are two categories of entrained flow gasifiers that are commercialized, the Dry-coal feed gasifiers and the coal water slurry-fed gasifier. These two will be presented here were the

SCGP represents the dry-fed and the Texaco process represents the slurry fed. Some other processes will also be discussed.

Shell Coal Gasification Process (SCGP)

This is a pressurized version of KT and was developed as a co-operation between Kopper and Shell. Two commercial plants are built so far as parts in ICGG plants. These have a production capacity of 2000 and 3000 tons per day. Shell has in addition several ongoing projects in China.

The SGCP is an up flowing gasifier meaning that the product gas leaves the reactor at the top. It is a dry-coal process so the feed has to be pressurized using a lock hopper. The coal is sized below 90μm and mixed with a transportation gas, normally nitrogen. The pressurized coal is than fed at typical four burners at the side walls where it reacts with oxygen. The reactions are fast (0.5-4 seconds) and bring along an up flowing syngas and a down flowing slag. The gasification temperature is about 1500°C and the pressure is 30-40bar. The product composition is typically two thirds CO, and one third H_2. There will also here be other substances as CO_2, CH_4 etc, but the production of CO and H_2 is maximized. An almost similar process is the so called Prenflo process. The SCGP and the Prenflo is often mentioned in the same descriptions [6].

The Texaco Process

The Texaco process was developed in the late 1940s mainly focused on natural gas. In the 1970s Texaco developed the technology to focus on coal gasification. Several plants for production of ammonia, methanol and town gas are placed in Japan, China and USA. The technology is also used in some IGCC units for instance the Polk Power Station in Florida [6].

The Texaco process is a slurry-feed gasifier were moist coal and oxygen enters at the top of the reactor. It is a down flowing entrained reactor were syngas and slag leave at the bottom. The feedstock is sized to about 100μm, slurried and pressurized with using a pump. The reactor pressure varies depending of it is a chemical plant or an IGCC facility. The slurry feed makes it possible to reach high pressure and for chemical application the pressure may be up to 80bar. For IGCC plants a typical operation pressure is about 40bar. The temperature is typically 1500°C [6].

The Texaco gasifier is the most inexpensive design on the market [6]. It is however very maintenance-intensive and to maximize production an extra standby reactor may be necessary. This will make the plant more expensive, so an economical calculation must be done to determine if it is a good investment all in all.

Recently the Texaco gasifier is better known as the GE gasifier when GE bought the gasification technology from Texaco.

Other gasifying processes

There are some other gasifying processes in the market, both older technology and brand new ones under construction. The Noell Process was developed by Deutsches Brennstoffinstitut Freiberg in 1975 and is better known under the name GSP. This is a dry-feed down flowing system with different variations of reactor design for different feedstocks.

The E-Gas Process is a two stage gasifier with coal-slurry feed. This gasifier handles low ranked coal and operating temperature at the first stage is 1400˚C. There are built a couple of IGCC plants in the USA using this technology [6].

There are two modern gasification processes recently developed in Japan for IGCC application. This is a gasifier constructed by Clean Coal Power R&D Company (CCP) and the gasifier is named the CCP Gasifier. The CCP combines the pressurized dry-feed technology with a two stage feeding using air as oxidant. In other word a combination of the SCGP and the E-Gas processes. The outlet temperature is about 1000˚C and the carbon conversion rate is closed to 100%. The other gasifier is under construction and is called the Eagle gasifier. This is a two stage gasifier using oxygen as oxidant and it has a high operation temperature at the first stage, 1600˚C [6].

Shell and the Texaco (GE) have most commercial experience on gasifiers, and these two processes are the most common around the world. They represent the two feeding processes and are therefore well usable examples of entrained flow gasifiers. The two processes have their advantages and disadvantages. The slurry fed Texaco gasifier can operate on very high pressure and the pressurizing system is simpler to handle than the Lock hopes system used in the Shell gasifier. In the other end it needs more oxygen. That both increases the energy consumption regarding to oxygen production and reduces the cold gas efficiency. The Shell

system requires less oxygen per produced amount of syngas but it can not operate on much higher pressure than 40bar. For IGCC applications this pressure is high enough. In addition is the oxygen consumption a considerably part of the total energy balance, so a minimum consumption is preferred. A high pressure is however profitably when it comes to CO_2 removal. About 40bar is anyway high since the molar fraction of CO_2 is over 0.3 after the gasification and shift reactor [6].

2.2.3.5   Feeding procedures for a gasifier

The gasification process operates at different pressure depending on the application area downstream the gasifier. For power production the gasification pressure normally lays in the range 20 to 40 bar [6]. A challenge for this kind of process is to feed the coal into an area with that pressure level. The problem occurs because of the fact that coal is a solid matter. Different techniques are developed to manage this duty. There are two approaches for pressurizing coal, Dry-Coal Feeding with Lock Hoppers and Pumping Coal as a Coal-Water Slurry [6]. The feed in a Dry-Coal gasifier is considered as dry, but in practice it will contain some humidity. This is not a problem for the gasification process since water anyway is a part of the gasification reaction

The Lock Hopper method is in short a three vessel system where each vessel operates at different pressure. They are connected to each other with valves and can be seen as a sluicing system. The solid matter is fed together with an inert gas from top at atmospheric pressure. The valve between the top hopper and the middle one (the lock hopper) is than open while the valve between the middle one and the bottom one is closed. After the lock hopper has been filled the upper valve is closed and the valve at the bottom is open. The pressure at the bottom hopper is high and the opening of the valve results in a pressure rise in the lock hopper.

In the Lock Hopper feeding method pulverized coal is fed with a transport gas often presented as nitrogen, syngas or carbon dioxide. For IGCC application nitrogen is the most common transport gas. Nitrogen is available from the air separation unit (ASU) and it will not affect the overall gasification efficiency considerable. The use of transport gasses makes it less attractive to rise the pressure in the gasification process when that results in a higher consumption of the given transport gas. Normally a dry-coal feed gasifier will not run at

higher pressure than 40 bar. This will not affect the case of IGCC while the pressure here normally is about 20 bar [6].

Pumping Coal as a Coal-Water Slurry is another method for pressurization coal. Slurry of coal and water is pressurized using a pump. This has its advantage on higher pressure rate and less advanced equipment than the Dry Feed Gasifyer. A slurry pump can deliver an outlet pressure as high as 200bar. This increases the capacity and higher pressure is also beneficial regarding to the CO_2 removal downstream the gasifier [20]. The disadvantages using this feeding technology is that it requires more oxygen since vaporization of water needs more heat.

2.3   Acid Gas Removal

2.3.1   Properties and technologies

Carbon dioxide and hydrogen sulfide are both products of a combustion or gasification process. CO_2 is produced from combustion of all kind of fossil fuels while to produce H_2S sulfur has to be present in the fuel. Different capture and storage technologies to avoid CO_2 emissions are presented and the more conventional process of H_2S removal is only quickly explained.

2.3.1.1   Chemical formation

Carbon dioxide is a natural end product in chemical and biological processes. It can not be considered as a toxic or acid gas. A complete combustion will always contain CO_2 as the final product. In a very simplified clean combustion of any fuel which contains carbon, the exhaust gas contains amounts of CO_2 dependent on fuel type. Carbon dioxide must be formed in order to release the full heat of combustion for a fuel containing carbon [3].

$$C_m H_n + \left(m + \frac{n}{4} \right) O_2 \Rightarrow m CO_2 + \frac{n}{2} H_2 O \qquad (2.49)$$

Equation 2.49 implies both for combustion of coal, oil, natural gas, biomass or any other fuel containing a hydrocarbon combination. It is therefore impossible to avoid formation of CO_2 in almost any kind of power production from combustion. There is nevertheless a great difference in the amount of carbon dioxide produced per energy unit liberated for the different fuels. Biomass is considered carbon neutral, while coal is considered to be the largest emitter.

Since CO_2 always is produced when fossil fuels are combusted, the solution to avoid, or at least minimize the emissions, is to capture and store it. There are many methods to do this and the collective term is CCS, Carbon dioxide Capture and Storage [2].

2.3.1.2   Combustion and capture methods

There are many technologies for both capture and storage of carbon dioxide. The technologies vary from research phase and demonstration plants to well-developed technologies.

Main capture technologies according to power production are post-combustion-, pre-combustion- and oxyfuel combustion capture [2]. In post-combustion CO_2 capture the carbon dioxide is captured from the exhaust gas after the combustion. The drawback of this technology is the relative low CO_2 concentration in the exhaust gas due to nitrogen in the air. Pre-combustion capture is CO_2 capture before the combustion. This is the method utilized in IGCC where fuel is transformed into a gas containing mainly H_2 and CO_2. The carbon dioxide is separated from the hydrogen before the hydrogen is sent to the combustion chamber. Oxyfuel combustion is combustion with pure oxygen instead of air. The exhaust gas from oxyfuel-combustion contains mainly water and CO_2 and the substances are easily separated by condensing the water. The drawback is the cost of producing pure oxygen and the fact that combustion with pure oxygen requires new types of turbines and technology.

A common drawback for all the capture technologies is the extra energy consumption required. As a rule of thumb, a power plant with CO_2 capture consumes about 15 to 30 percent more fuel to produce the same amount of electricity and heat as an equal plant without capture facilities. This equals a reduction of 7 to 15 percent points in efficiency [16] [21].

The most explored and most likely to be the common storage technology in the future is geological storage. This may be done by storage in empty gas or oil fields or in saline formations. It is also possible to use CO_2 to increase the pressure in oil fields by Enhanced Oil Recovery (EOR). In addition to store carbon dioxide this technology increases the production from a well. Another technology with a large potential in the future is deep sea storage. The ocean is capable to receive great amounts of carbon dioxide and keep it there [2].

As mentioned above, IGCC with CO_2 capture utilizes pre-combustion capture technology. It is of cause possible to use post-combustion technology in an IGCC plant, but this gives a remarkable energy efficiency reduction. In the subsequent part the different methods to separate the hydrogen and carbon dioxide is looked further into. The issue of storage is independent of capture technology and storage location is not further discussed in this report.

2.3.2   Removal of H₂S and CO₂

Acid gas removal is in IGCC context originally removal of hydrogen sulfide, H_2S. In IGCC plants with CO_2 removal, capture of carbon dioxide is included in the acid gas removal. The capture of H_2S and CO_2 are either done simultaneously in one operation or split in two separate units.

The H_2S may be captured before or after the water gas shift reactor while CO_2 has to be captured after the shift reactor. Removal of carbon dioxide before the shift reactor is in fact not possible because the CO_2 is not yet produced. This is because the carbon bound in CO in the syngas needs to be bound to CO_2 before it is removed. The conversion from carbon monoxide to carbon dioxide happens in the shift reactor and the CO_2 remove must therefore be done after this process.

By removal of H_2S together with CO_2 after the shift reactor the shift process is called "sour water gas shift". This is because the acid H_2S is still in the syngas when the syngas enters the shift reactor. A sketch of the stages in transforming coal into a H_2 rich gas in a sour water gas shift reaction is shown in figure 2.21.
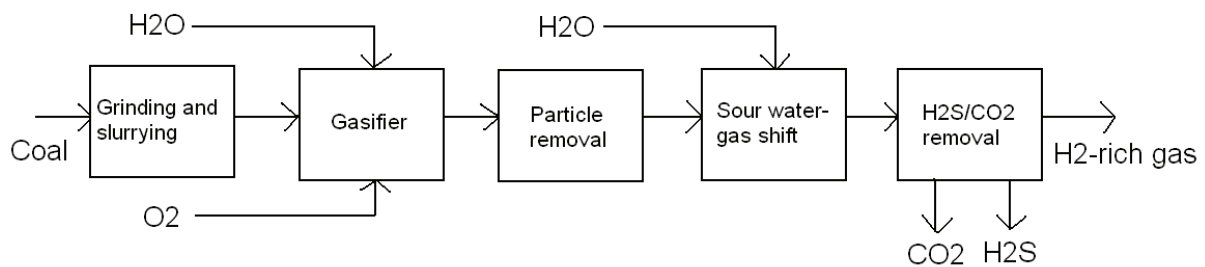
Figure 2.21. Sour water gas shift reaction [16].

The alternative is to remove the H_2S before the shift reactor. CO_2 must as mentioned be captured after the shift reactor and the removal processes are therefore completely separated. This is called "sweet water gas shift" because the acid H_2S is removed before the shift reactor. A corresponding figure as for the sour water gas shift reaction is shown for sweet water gas shift reaction in figure 2.22.
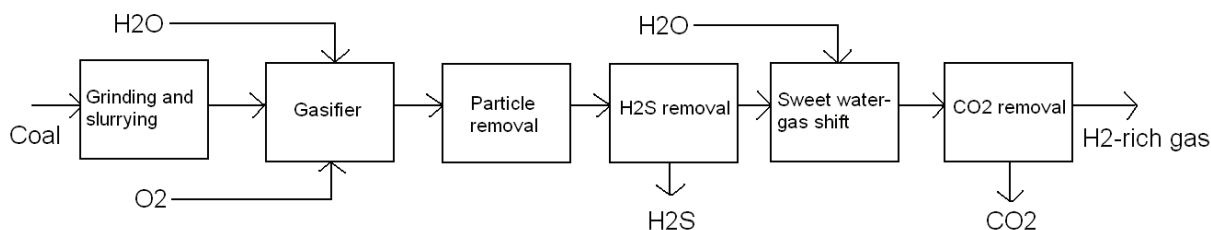
Figure 2.22. Sweet water gas shift reaction [16].

In the subsequent sections an introduction to the capture technologies for CO_2 and H_2S removal are presented.

2.3.2.1 CO_2 capture technologies

Capture of CO_2 is a very wide field and there are many different technologies available. In an IGCC plant the CO_2 should be separated and removed from the H_2 before the fuel is sent to the turbine. For separation between CO_2 and H_2 the most common technologies are absorption, adsorption, membrane process and cryogenic process [21]. What technology to choose is very much dependent on the partial pressure of CO_2, but the decision may vary from plant to plant.

Absorption

Absorption is to attach the CO_2 to a liquid solvent and remove the solvent from the fuel gas. Another often used word for adsorption is scrubbing. With absorption in a liquid solvent high purity levels and separation factors may be achieved. In general absorption is preferred for separation between H_2 and CO_2 when the partial pressure of CO_2 is high [21].

Absorption is divided into three main types, physical absorption, chemical absorption and the combination of these, physical –chemical absorption. The difference between the types of absorption is not further studied, but normally has physical scrubbing a slightly lower energy demand than chemical scrubbing. The energy demand is not remarkable different and a rule of thumb is that physical absorption is more energy efficient for pressures over 10 bar. The energy demand is in both cases about 0.04 to 0.09kWh per kilogram of carbon dioxide removed [21].

After the liquid solvent is removed from the fuel gas the CO_2 is removed from the solvent. This is done to regenerate the solvent. How to remove the carbon dioxide from the solvent depends on what kind of absorption method used. For physical scrubbing the solvent with CO_2 must be expanded and for chemical scrubbing it must be heated. For physical-chemical absorption the solvent is regenerated by a combination of pressure drop and increasing temperature. This correlates with the rule of thumb that high pressure fuel gas gives incentives for physical absorption.

Adsorption

As the word indicates adsorption has similarities with absorption. While absorption is to attach the carbon dioxide to a liquid solvent, adsorption is to attach the CO_2 to a solid solvent.

Also adsorption is divided between physical and chemical with a corresponding difference for regenerating of the solvent. Physical adsorption has regeneration through pressure drop, chemical adsorption has regeneration through a temperature swing and physical-chemical adsorption has a combination of pressure drop and increasing temperature.

Adsorption has an energy demand of 0.16 to 0.20kWh per kg CO_2 removed and requires very large equipment. It is therefore only suitable for some occurrences with small gas streams [21].

Membrane processes

A membrane separates H_2 and CO_2 by slipping one of the gases through and letting the other one stay behind. As a general rule is it easier to let gases with small molecular weight through the membrane than heavier molecules. Hydrogen has a remarkable lower molecular weight than carbon dioxide and CO_2 removal from the fuel gas is in this case therefore hydrogen removal. Although, the hydrogen stream let through the membrane is off course the utilized product for power production.

The main energy losses with membrane processes are the pressure drop between the two sides of the membrane and H_2 losses in CO_2 stream. Hydrogen in the waste CO_2 stream leads to lesser fuel fed to turbine per amount of coal fed to the gasifier.

Membrane processes has an energy demand of about 0.17 to 0.29kWh per kilogram of carbon dioxide removed [21].

Cryogenic processes

A cryogenic process removes the carbon dioxide by direct condensation, sublimation or distillation. This may be done with or without a solvent, but no solvent require low temperature or high pressure.

Direct condensation with no solvent requires 88bar at -56°C and at 0°C the pressure must be minimum 592bar to condensate the carbon dioxide. This is to energy demanding to be economic feasible.

Below the triple point of carbon dioxide of -56.6°C gaseous CO_2 sublimes direct into solid state. Exxon has designed a commercial process for CO_2 freezing called Controlled Freezing Zone (CFZ). This process operates at 4bar with a temperature of -100°C and for a 90% capture ratio the energy consumption is about 0.37kWh per kilogram of CO_2 removed [21].

2.3.2.2 H_2S capture technology

Removal of hydrogen sulfide is done by converting the H_2S into elemental sulfur, S. To do this the hydrogen sulfide reacts with oxygen forming elemental sulfur and water. The reaction is shown in equation 2.49.

$$H_2S + 1/2O_2 \rightarrow S + H_2O \qquad\qquad (2.49)$$

This is called the Claus process and was discovered for the first time about 100 years ago. Today it is the standard hydrogen sulfide removal procedure used in H_2S scrubbers [22].

The Claus process is equal even if the H_2S scrubber is placed before or after the water gas shift reactor.

2.4 Power Island

2.4.1 Introduction

The gasification products can be used in several industries. In this report there will be focused on the use of syngas as fuel in power plants, IGCC. There are mainly two different fuels that are relevant for IGCC plants depending if it is with or without CO_2 capture. A power plant without CO_2 capture can use a mixture of CO and H_2 from the gasifier as fuel. That differs from plants with CO_2 capture where the syngas goes through a shift reactor where conversion to CO_2 and more H_2 occur. This results in a high partial pressure of CO_2 which can be removed relatively easily. The heating value part of the fuel will then exists of H_2 only in addition to some traces of CO.

The power island in an IGCC has roughly the same principles as other combined cycles where power is generated in a gas cycle and a steam cycle. Compressed air and fuel are fed to the gas turbine where combustion occurs and chemical energy is converted to mechanical energy. The exhaust gas from this process is again used to run the steam cycle.

The gas cycles performance depends on the turbine inlet temperature (TIT) and the mass flow. A higher inlet temperature at the turbine gives a higher temperature drop, which again directly affects the change in enthalpy. There are however restrictions in how high the temperature can be caused by the protection of the materials. A higher mass flow also increases the power output, but also here there are limitations. These will be discussed more in *2.4.2 Turbine fired with syngas*.

The exhaust gas from the gas turbine is used to produce steam. Typical exhaust temperature is 450-650˚C and much of the energy in the exhaust gas can therefore be recovered in a heat recovery steam generator, HRSG. In a HRSG high pressure vapor is produced at 30-120bar with temperatures in the range of 450-560˚C. The high pressure water vapor is used in a steam turbine to generate more power. The output pressure is typical 0.03-0.07bar [19]. After the steam turbine the mixed phase flow enters a condenser which condenses the remaining vapor, making the water ready to be pumped up to the mentioned high pressure. The high pressure

water enters the HRSG and the cycle starts over. The exhaust gas is through the HRSG cooled to 80-200˚C dependent on the size and technology of the equipment [21]. In addition to the exhaust gas, steam can also be generated from the heat liberated in the gasification process. The overall efficiency will then increase.

In a combined cycle power plant, the gas turbine usually contributes to about 2/3 of the total power production and the steam turbine contributes to the remaining 1/3 [21]. When designing combined cycles it may be a helpful rule of thumb to check if the ratios are in the mentioned areas.

For both syngas fueled and H_2 fueled turbines there are challenges compared to natural gas fired power plant, NGCC. A short introduction to syngas and H_2 fired gas turbines will be given here. There is more available theory about syngas turbines than about H_2 fired equipment. Hydrogen fired turbines is still not a very conventional technology.

2.4.2 Turbines fired with syngas

2.4.2.1 Turbine conditions

In traditional gas turbines the fuel is premixed with air to lower the peak flame temperature and to reduce the formation of thermal NO_X. Hydrogen has a high flame propagation speed and therefore the pre mixing is not useful for syngas turbines. There is a danger of flashback caused by the properties of the hydrogen [20]. For IGCC application dilution of the fuel is a method for temperature and NO_X control. Typical diluters are nitrogen and water steam. An advantage for IGCC plants are the availability of N_2 from the air separation unit.

The fuel in gas fired power plants are usual a mixture where methane is the major component. Methane has a lower heating value (LHV) of about 800MJ/kmol [19]. Mixtures of CO and H_2 have a corresponding value of about 250MJ/kmol depending on the distribution between the substances. A product stream from a gasifier also contains other substances without heating values. This bring along an even lower volumetric LHV. The volumetric heating value for syngas is in literature often set to only 25% of the natural gas. The consequence of this is that a syngas turbine requires about four times higher fuel flow rate to maintain the same turbine

inlet temperature [20]. Higher flow rate increases the power output but it can also contribute to problems for existing turbines. This can be explained using the equation of continuity 2.50 and the ideal gas law 2.51 [16].

$$\dot{m} = \rho u A_c \tag{2.50}$$

$$p = \rho \frac{R}{M} T \tag{2.51}$$

With constant speed u, equation 2.52 is formed by rearranging equation 2.51 and combine it with equation 2.50.

$$\dot{m} \sim \frac{Mp}{RT} A_c \tag{2.52}$$

$\dot{m}$ =   flow rate

M =   molar weight

p =   pressure

R =   the universal gas constant

T =   temperature

A_c =   cross section flow area

ρ =   density

The relation in 2.52 can be expanded to give the relation between a known standard condition and another condition.

$$\frac{\dot{m}}{\dot{m}_{ref}} = \frac{M}{M_{ref}} \frac{p}{p_{ref}} \frac{R_{ref}}{R} \frac{T_{ref}}{T} \frac{A_c}{A_{c,ref}} \tag{2.53}$$

If the p and the T represent the inlet pressure and the inlet temperature of the turbine, one can from this equation see the relation for a given fuel (the same M) and a constant cross section area. Increasing in the flow rate will then either reduce the inlet temperature or increase the inlet pressure for the turbine. The TIT is however supposed to be kept as high as possible so the increasing in pressure is the main consequence of increasing the mass flow [20]. The inlet pressure of the turbine is assumed to be the same as the outlet pressure of the compressor. A higher mass flow may ergo increase the back pressure at the compressor so much that it goes into surge. When a compressor is surging the back pressure is higher than normal and the

pressure rate decreases. This will again reduce the air flow through the compressor [20]. When this occurs depends on the compressor surge margin which depends on the turbine type.

Another problem that may occur with syngas fuel is that the increased mass flow increases the power output. This will directly raise the torque and the rotors have to handle with this higher force.

When handling with natural gas compared to syngas the molecular weight M will also differ. Pure methane has a molecular weight of about 16.04kg/kmol and a mixture of CO and H_2 will typically has a corresponding value of about 20kg/kmol. These numbers will differ a bit in real life since natural gas is not pure methane and the syngas mixture also contains other substances.

It should be mentioned that in a gas turbine the fuel is mixed with air with a fuel/air ratio in the range of 0.02 for a typical natural gas fired turbine [23]. These numbers are calculated on mass basis. That implies that the dominating part for the mass flow and the total molar fraction is the air. A syngas fueled turbine requires a much higher fuel/air ratio. The volumetric LHV for syngas is as mentioned about 25% of methane. The fuel/air ratio operates on a mass basis and therefore other factors also affect the fuel/air ratio for a syngas fueled turbine. The molar weight is higher and the need of inert gasses also contributes to a higher fuel/air ratio. A large gas turbine can have an air flow of about 600kg/s. The total mass flow through the turbine will for a natural gas fired turbine be given in equation 2.54.

$$600 + 600 \cdot 0.02 = 612 \left[\frac{kg}{s} \right] \tag{2.54}$$

For a syngas fired turbine with a fuel/air ratio assumed to be 0.12 the equivalent value is given by equation 2.55.

$$600 + 600 \cdot 0.12 = 672 \left[\frac{kg}{s} \right] \tag{2.55}$$

From these relations one can see that the mass flow through the turbine will increase with about 10% when the fuel is changed from natural gas to syngas.

2.4.2.2   Modification of the equipment to handle syngas

A method to avoid surging is to increase the cross sectional area to handle a higher flow rate. There is also a possibility to add an extra compressor stage. Then the equipment can operate on a higher overall pressure ratio and avoid surge problems [20].

Another method is to integrate the gas turbine with the air separation unit. One can then take some of the compressed air and send it directly to the ASU. Some of this air can be compensated with nitrogen from the ASU. If the N_2 flow is lower than the amount of air taken from the compressor, the overall mass flow is reduced. This technology is used in the Buggenum plant in the Netherlands [20].

2.4.3   Turbines fired with hydrogen only

One of the main challenges for IGCC plants with CO_2 capture is to get turbines running on hydrogen only. H_2 turbines will reach a high temperature which is damaging for the materials. It also has the case of moisture in the exhaust gas that also contributes to thermal challenges caused by the physical properties of water [20]. Water has a high heat capacity, and a high amount of water will increase the heat transfer in the turbine and put more strain on the materials. Cooling is required to reduce the NO_X formation. Use of water for cooling purpose will increase the amount of moisture even more.

Recent developed turbines seem to handle with diluted hydrogen as fuel. Siemens has for example their type SGT6-5000F that according to their report handles both syngas and hydrogen [24]. This turbine has been tested for different fuel compositions and the results are shown in table 2.7.

Table 2.7. Test results SGT6-5000F [24].

Vol%	Syngas		H_2	
	min	max	min	max
H_2	11 %	22 %	30 %	73 %
CO	12 %	34 %	0 %	46 %
CO_2	1 %	11 %	0 %	14 %
CH_4	0 %	4 %	0 %	5 %
N_2	5 %	41 %	0 %	60 %
H_2O	0 %	57 %	0 %	57 %

Table 2.7 shows that this turbine can handle a fuel with a molar fraction of H_2 at 0.7 and even higher. A mixture of H_2, N_2, some CO and CO_2 will be a typical composition for this turbine. It should be noted that SGT6-5000F is a 3600RPM turbine. It is therefore constructed for 60Hz line frequency. In Europe the power grid operates at 50Hz and it therefore requires a 3000RPM turbine. For this frequency the SGT5-4000F is the equivalent to the SGT6-5000F. This turbine type is used at the syngas fired IGCC plant at Puertollano in Spain [20]. A corresponding adjustment as for the 60Hz turbine can probably be done for the 50Hz turbine to operate with diluted hydrogen as fuel.

2.5   IGCC plant

2.5.1   Integration of processes

As mentioned in *1.3 Integrated Gasification Combined Cycle* in the introduction, the four previous main processes are supposed to be set together in a total IGCC power plant. The different processes are integrated and achieve mass flows from each other. They should also be heat integrated to utilize possible heat or coldness surplus between the islands.

2.5.1.1   Mass flow

The oxygen produced in the ASU is used in the gasification island together with coal and steam. The gas out of the shift reactor is cleaned for H_2S and CO_2. The H_2 rich fuel is now mixed with nitrogen separated from the oxygen in the ASU, before the fuel is sent to the combustion chamber in the power island. An overview of this process is given in figure 1.3.
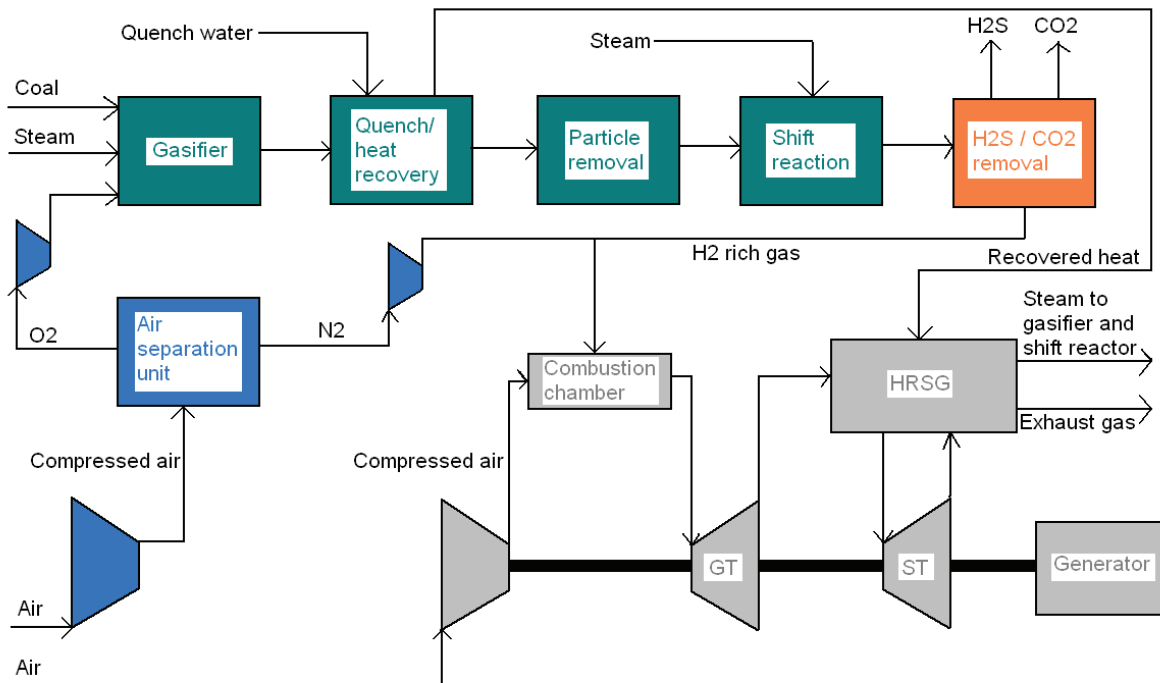
Figure 1.3. Overview of the main processes in an IGCC Power Plant.

The figure describes the mass flow between the separate units and the four islands.

2.5.1.2 Heat flow

In addition to the flow of mass between the separate islands it is also important to integrate need of heat and cooling. Quench water is needed between the gasifier and shift reactor. The heat taken out of the syngas at this point may be recovered in the HRSG. All the compressors, both in the Air Separation Island and the Power Island, need aftercooling to minimize energy consumption. The heat removed here is also possible to integrate and utilize. It may be used to produce steam in the HRSG or to preheat oxygen or coal entering the gasifier. The need of steam in the gasifier and shift reactor is also covered internally by receiving steam from the HRSG. There is also a possible need of heat in the acid gas removal dependent on CO_2 capture method.

An overview of main needs of heat and coldness in an IGCC plant are given in table 2.8. There may be other important heating or cooling requirements in a plant, but the major duties that should be covered are mentioned.

Table 2.8. Expected heat and cooling integration.

Need of heat	Need of coldness
Preheat of oxygen before gasifier	Aftercooling in main air compressor in the ASU
Preheat of coal before gasifier	Quench water after gasifier
Steam to gasifier	Aftercooling in nitrogen compressor
Steam to shift reactor	Aftercooling in compressors in the power island
(CO_2 capture unit)	Quench water in steam cycle

The table is not balanced and the total need of heat and coldness are not necessarily equal. It is important to remember that heating or cooling to ambient temperature not needs to be covered internally and can be done by ambient air.

2.5.2   *Energy efficiency*

Energy efficiencies in IGCC plants are not easy to find. Involved companies are careful with information sharing and many technologies are considered company secrets. Efficiency information available is mainly given by independent non-commercial organizations like IPCC and IEA.

To calculate the total efficiency of an IGCC plant with CO_2 capture, all the processes in the power plant must be included. If it is assumed that the plant only generates electricity and do not produce heat for external use equation 2.56 gives the total plant efficiency [19].

$$\eta_{plant} = \frac{W_{net}}{Q_{in}}$$
(2.56)

W_{net} is the net electricity production of the power plant and Q_{in} is the total heating value of the fuel fed to the plant.

To calculate W_{net} a total energy analysis of the plant must be done. W_{net} equals the electricity output from the generator minus all internal electricity demands. This mainly different compressor and pump work. Q_{in} is the lower heating value (LHV) of the fuel multiplied with the amount fed to give the specific W_{net}.

According to IPCC, a new IGCC plant with CO_2 capture has typical an efficiency around 35%. Future IGCC plants of this kind may although have efficiency up to 40 percent [2]. This is supported by the U.S Department of Energy saying the plant efficiency dependent on technology utilized and capture ratio is ranging from around 30 to 38 percent. A typical IGCC plant with relative high CO_2 capture ratio and optimal combination of gasifier and capture method is in the area of 36% [21].

3 Method

3.1 Air Separation Island

3.1.1 Simulation tool

The air separation island is modeled in PRO/II 8.0 by Simsci-esscor. The model is used to calculate the energy cost of producing oxygen to the gasifier and nitrogen to dilute the fuel before the Power Island. The needed amount of oxygen depends on the type of gasifier and type of coal used. The need of nitrogen is not as accurate as the need of oxygen. Nitrogen is used as a diluter and the amount mixed with the fuel is only regulating the heating value of the fuel fed to the gas turbine. In the method part of the report the amount of oxygen and nitrogen operates in percent of one mole of air. The modeled production of oxygen and nitrogen are therefore measured in mole percent.

To model the air separation unit a lot of optimization and adjustments where continuous made. This is done mainly by manually iteration. Only the major changes are presented in the report, small adjustments and iteration steps are not shown. The final model shown in *4.1.1.6 Overall GOX considerations* is although not changed after presented.

Ambient conditions are set to 298K and 1bar.

3.1.2 Gaseous oxygen

An air separation unit is modeled by stepwise expansion and manual iteration. The GOX model is presented similar as the plant in *2.1.2 Air separation unit* in the theoretical background. The presentation of the model is following the air, oxygen and nitrogen streams chronological and not the stepwise and iterating development of the model.

3.1.2.1   Compression

The compressor work is the only external energy input to the Air Separation Island. Cooling water may also be looked upon as an external energy demand, but this is described in *3.1.2.3 Air cleaning*. It is by this important to minimize the work done by the main compressor.

In figure 2.7 in *2.1.2.1 Introduction* the compressor is drawn as one large unit. To have one compressor handle the whole lifting work is very energy ineffective. The use of energy falls with an increasing number of compressors. The head on each compressor is reduced and the total work decreases. To decide the optimal number of compressors the relationship between reduced energy input of including one extra compressor and the investment cost of this extra compressor must be studied. This is done in *4.1.1.4 Investment cost considerations*. It is decided to use 4 compressors and in the following sections the models are presented like this.

The compression rate is decided from the pressure level in the columns. The pressure in the columns is further decided by the temperature difference in the combined condenser and reboiler. A pressure loss in the aftercoolers, the molecular sieves and the main heat exchanger has to be added on to the feed pressure to the high pressure column. The pressure in the bottom of the high pressure column is initially set to 6bar. To handle a high pressure column feed pressure of 6bar, the compressors are set to deliver air at 6.43bars. How the pressure loss distributes between the units before the HP column is explained when the unit is looked into.

The polytrophic efficiency was for the compressors set to 85 % [10].

3.1.2.2   Air cleaning

After compression and aftercooling the compressed air is cleaned for carbon dioxide and moisture in the molecular sieves. Molecular sieves remove the unwanted substances by adsorption and are not easily modeled in PRO/II. The water vapor and carbon dioxide are therefore left out of the model and the pressure loss in molecular sieves is included in the pressure loss in the main heat exchanger. Table 3.1 shows the simplified air composition used in the model. The composition presented is not as accurate as the composition presented in table 2.1, but the small derogation has neglectable impact on the air separation model

Table 3.1 Dry air composition used in the ASU model.

Component	Volume percent
N_2	78.1
O_2	21.0
Ar	0.9

To get the right outlet amount of the nitrogen and oxygen stream from the air separation island the air feed is set to 0.99 instead of 1.00. This is to adjust for the water vapor removed in the molecular sieves. If 1kmol/s of air with moisture level of 1 molar percent is fed to the molecular sieves 0.99kmol/s of dry air leaves the sieves.

Because of the air feed reduction of 0.01kmol/s, the compressor work is also reduced. This leads to a small energy input reduction which exists only in the model. This reduction has to be taken into account when the Air Separation Island is discussed.

Figure 3.1 shows the 4 compressors and table 3.2 and 3.3 respectively gives the compressor and stream properties.
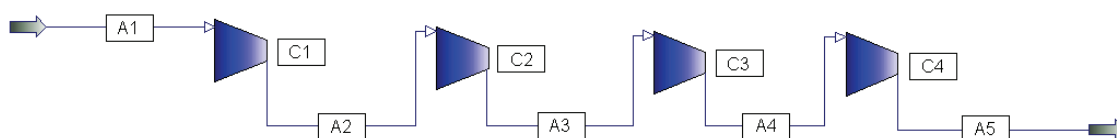
Figure 3.1. Model of air compressor.

Table 3.2. Compressor work of compressing 0.99 kmol of dry air.

Compressor Name			C1	C2	C3	C4
Pressure	bar		1.60	2.50	4.00	6.43
Temperature	K		348.94	348.39	351.33	351.91
Head	M		5224	5167	5468	5526
Actual Work	kW		1469	1453	1538	1554
Isentropic coef.. k			1.4013	1.4024	1.4041	1.407

Table 3.3. Stream properties of air.

Stream Name			A1	A2	A3	A4	A5
Phase			Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K		298	298	298	298	298
Pressure	bar		1.000	1,570	2,450	3,920	6,300
Flowrate	kmol/s		0,990	0,990	0,990	0,990	0,990

By comparison between table 3.2 and 3.3 the relationship between the aftercoolers and the aftercooler pressure drop is given. Stream A2 compared with compressor C1 is used as an example. In C1 the pressure is 1.6bar and the air temperature is about 349K. Out of the compressor stream A2 is at 298K and 1.57bar. This is equal to cooling to 25°C with a pressure loss of 0.03bar. The pressure drop in the aftercoolers is set to 2-3 percent of the previous compressor pressure outlet.

Compressor work is mentioned as the only energy input in the ASU model in *3.1.2.1 Compression*. Cooling of the air in the compressors is an external energy demand and is also an energy input. For a plant located by the ocean or in northern Europe cooling to 25°C is normally calculated as free. In warmer parts of the world or in the inland cooling may be an additional and quite expensive energy demand. To assume compressor work as the only energy input may in some cases therefore be considered as wrong. In this report the ambient temperature is 25°C and cooling to this temperature is not given any energy cost.

3.1.2.3   Main heat exchanger

The main heat exchanger is modeled as to simple heat exchangers, E1 and E2. They respectively exchange heat with the nitrogen and oxygen stream. To have optimal regulation opportunities in the model and to avoid cross pinch exchanging the heat exchangers are placed in parallel in stead of in series [25]. The compressed air before the main heat exchanger is split in two and led to different heat exchangers. This is shown in figure 3.2.
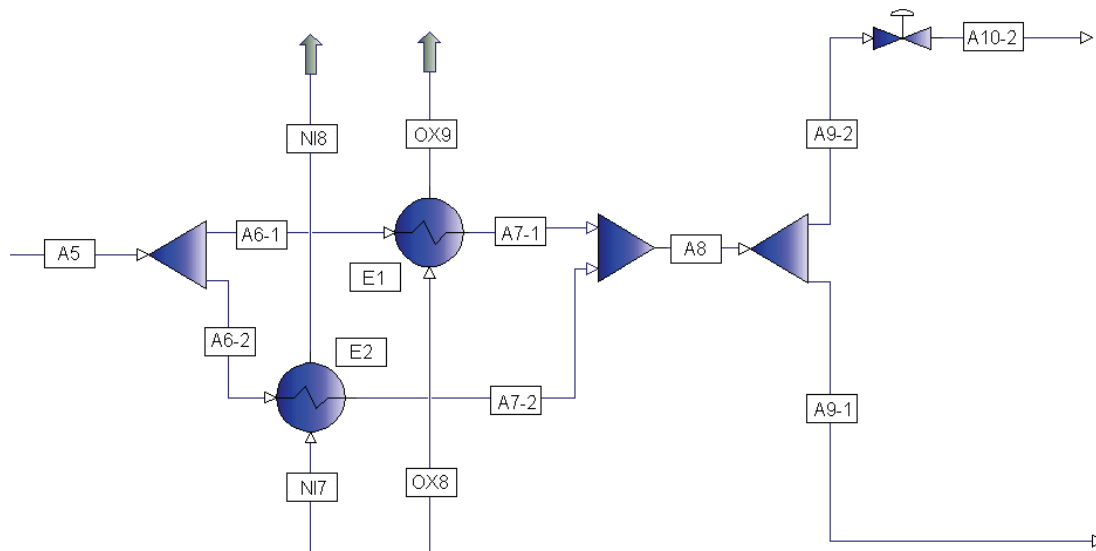
Figure 3.2. Model of the main heat exchanger.

To have optimal heat exchanging between the cold inputs OX8 and NI7 and the hot inputs A6-1 and A6-2, the cold output temperatures both has to be as close to the temperature in stream A5 as possible. Stream A5 is coming from the aftercooler and holds ambient temperature. Calculating with a ΔT of 1K, OX9 and NI8 should optimally be heated to 297K.

Stream A-5 entering the main heat exchanger has a defined pressure. Through the exchanger the there is a certain pressure drop. As mentioned in *3.1.2.2 Air cleaning* there is also a pressure drop in the molecular sieves not yet taken into account. In the modeled main heat exchanger are the pressure drop of the molecular sieves and the heat exchangers considered together. The total drop in these two processes is set to 0.3bar, which equals a pressure reduction of 4.8 percent.

The stream taken out of the heat exchanger and fed to the low pressure column is in figure 3.2 taken out after the heat exchanger. This is done since the model is able to cool the entire air feed without taking out A9-2 in the middle of the exchanger. If A9-2 is taken out earlier it is possible to cool the nitrogen stream lower than ambient temperature and by this achieve a higher efficiency in the Power Island. A discussion about this is presented in *4.1.1.3 Change in the main heat exchanger*. Stream A9-1 is at the wanted pressure of the high pressure column, while stream A9-2 has to be choked to fit the low pressure column.

Since air is a non ideal gas, choking between A9-2 and A10-2 causes a temperature fall in the stream [19]. The choking is done in a valve and adjusts the pressure to low pressure column pressure. The pressure may also be reduced by an expander. An expander will lead to an even lower temperature at A10-2 and does also produce a small energy amount that may be utilized. Use of valve or expander is also closely connected to the topic of where in the heat exchanger A9-2 is taken out. As mentioned above, a closer analysis of this is presented in *4.1.1.3 Change in the main heat exchanger*.

3.1.2.4 High pressure column

Stream A9-1 enters the bottom tray of the high pressure column at 6bar. The column has a pressure drop upwards the column and the pressure drop is set to 0.5bar. The condenser in the column makes it advantageous to specify the nitrogen purity in the stream leaving the condenser. This purity is set to be 99 percent and the condenser duty is varied by PRO/II to achieve this. At the bottom of the column an oxygen rich stream leaves the column, but no specifications of purity or mass rate are made for this stream. The mentioned pressure assumption gives a pressure at 5.5bar in the top stream and 6bar in the bottom stream.

It also has to be decided on how many trays needed to achieve the wanted separation. To decide the tray number the column is initially set to have 40 trays. This is probably too many trays, but with a conservative assumption it is easier to adjust the number of trays to an optimal level afterwards. Figure 3.3 shows the separation factor plotted against the number of trays. The figure is plotted in PRO/II.
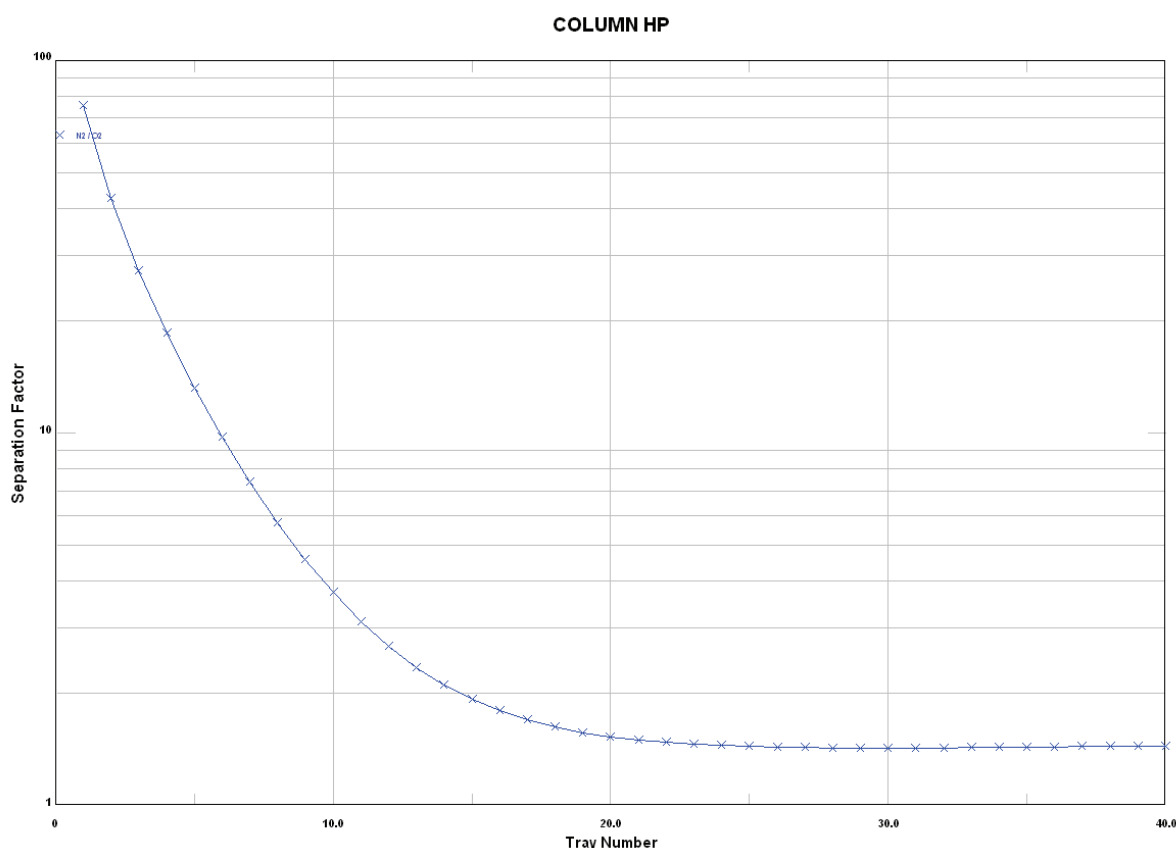
Figure 3.3. Separation factor for the high pressure column.

The figure shows the separation between nitrogen and oxygen for an increasing number of trays with a PRO/II calculated condenser duty for a specific purity level. To the left in the figure the separation with only one tray is shown. For an increasing number of trays the separation between nitrogen and oxygen increases. The separation converges towards a specific level where an increase of trays does not lead to a considerable higher purity.

The number of trays needed at a specific purity level is directly connected to the duty of the condenser. If the number of trays is reduced the purity level may be maintained if the duty is increased. Since the wanted purity level is specified in the column, the graph shown in figure 3.3 is changed if the number of trays is changed. If the column did not have the purity level specification and the condenser duty was constant instead, the graph would not change if the number of trays where changed. Then the number of trays would be the decisive separation variable. The differences in the graph with changed number of trays are therefore caused of the variation in condenser duty.

The condenser in the high pressure column is reboiler in the low pressure column, and the number of trays in the two columns is therefore affected by each other. A closer analysis of need of trays in both the columns is made in *4.1.1.4 Investment costs considerations*.

A model of the high pressure column is shown in figure 3.4. Here are the column shown with the initial 40 trays, but this is changed in the final model.
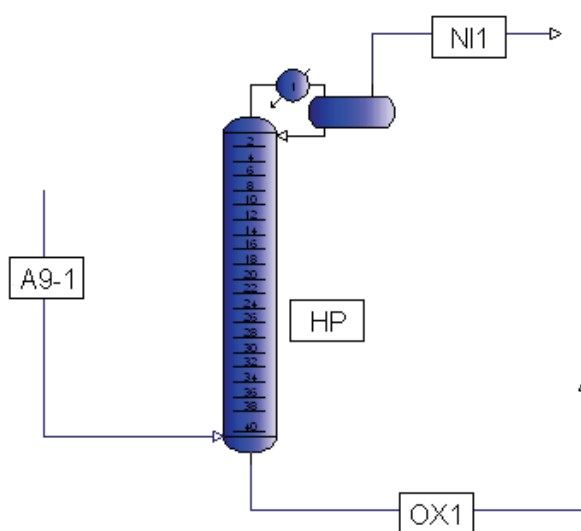
Figure 3.4. Model of high pressure column.

3.1.2.5   Low pressure column

The low pressure column has several incoming feeds. Stream NI1 from the condenser in the high pressure column is cooled and choked and enters the low pressure column at the top tray. This stream is named NI5. Stream OX1 from the high pressure column is choked and fed to the mid tray of the low pressure column. The stream name is OX2. Moving the feed tray of OX2 will have some minor impacts on the purity level of outgoing streams of the low pressure column. This may be done if the column should be extremely optimized or needs a very accurate purity level.

In addition to the feeds from the high pressure column the low pressure column is fed with the small earlier mentioned air feed named A10-2.

In the model there is a stream of distilled oxygen lead out at the bottom tray of the low pressure column. This stream is at a fixed rate and is specified to contain a specific amount of oxygen. The purity level is set to 95% and stream is called OX6. The rest of the oxygen

mixture in the bottom of the column is sent to the combined condenser and reboiler in stream OX3.

The pressure in the bottom of the column is set to 1.5bar. This is a level based on minimum temperature approach in the combined condenser and reboiler. This is further explained in *3.1.2.6 Combined condenser and reboiler*. With a pressure drop of 0.5bar through the column the nitrogen leaving the top of the column is at 1 bar. The feeds to the column have to be adjusted by choking to the pressure level at the tray where they are fed.

A figure of the low pressure column is shown in figure 3.5. In this figure the combined condenser and reboiler shown as heat exchanger E6. This unit will be closer explained in the subsequent section *3.1.2.6 Combined condenser and reboiler*.
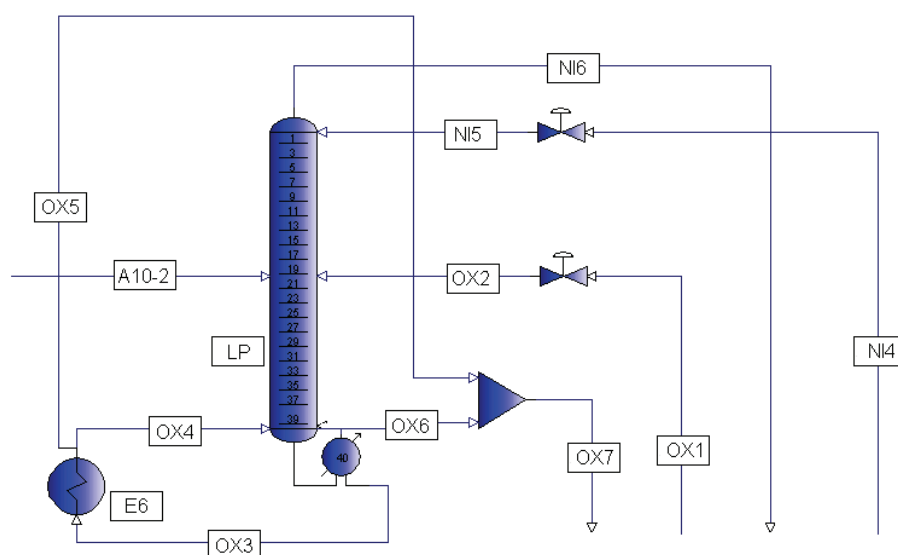
Figure 3.5. Model of low pressure column.

As mentioned in *3.1.2.4 High pressure column*, the number of trays in the two columns is closely connected. The need of trays in both the columns is discussed in *4.1.1.4 Investment costs considerations*.

3.1.2.6 Combined condenser and reboiler

The combined condenser and reboiler (CCR) is in PRO/II modeled as an attached heat exchanger. The bottom stream from the low pressure column is sent to a reboiler integrated in

the column. The low pressure column needs a variable to operate and converge and the integrated reboiler has this purpose. The reboiler is only included in the model for operational reasons and has in the final model a neglectable duty.

After the integrated reboiler with neglectable duty, stream OX3 enters the actual CCR modeled as heat exchanger E6. E6 is attached to the HP column and in E6 the cold stream OX3 is boiled with heat from the condenser in this column. The cold outlet of the exchanger is split in two streams containing respectively the vapor and liquid phase of the outlet. OX4 is in vapor phase and sent back to the bottom tray of the low pressure column while the liquid OX5 is completely distilled oxygen sent towards the main heat exchanger.

OX5 has equal phase and purity level as OX6 and they are mixed before used in cooling purposes. The mix is called OX7 and represents the total oxygen production of the Air Separation Island.

In figure 3.6 the model of the combined condenser and reboiler is shown.
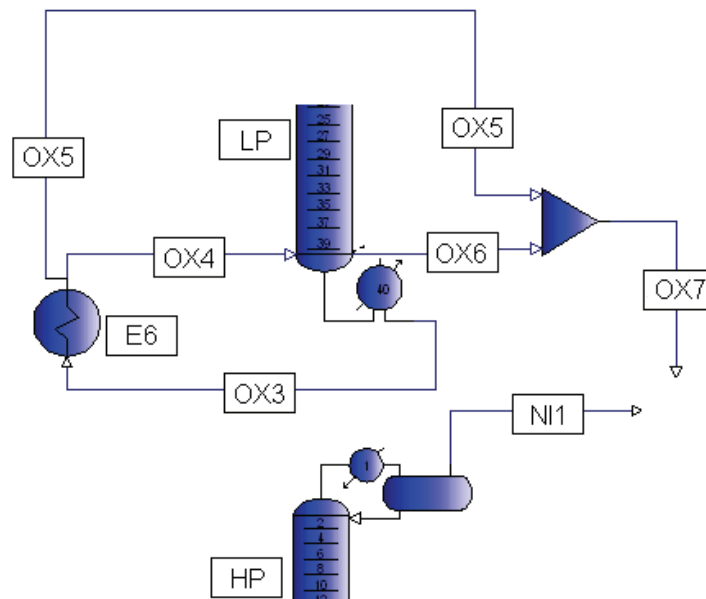
Figure 3.6. Model of combined condenser and reboiler.

In PRO/II there are two ways to connect the heat exchanger modeled as reboiler in the low pressure column to the condenser in the high pressure column. The first is to use the *Attach to column* function on the hot side of the heat exchanger. The cold side is defined by streams in and out of the heat exchanger. This function connects the duty of the condenser in the high

pressure column to the duty delivered on hot side of the exchanger. The other is to define a FORTRAN subroutine in the specification of the heat exchanger. In the modeled developed for this report the Attach to column function is used.

When using the Attach to column function it is important to be aware of the minimum temperature approach, ΔT. The Attach to column function only use the duty in the condenser to boil stream OX3 without concerning about temperatures. A model with heat transferred from cold to hot side would therefore be operational in PRO/II with this function. This is not legal according to the second law of thermodynamics and the temperature difference needs to be taken care of manually. With a ΔT value of 1K the stream OX3 always has to be 1K below the temperature out of the condenser. This temperature is equal to the temperature of NI1. For the island to be operational in real life NI1 must always be at least 1K above OX3.

The parameters deciding the temperature of NI1 and OX3 is the top pressure of the high pressure column and the bottom pressure of the low pressure column. NI1 is directly dependent on the pressure in the condenser as long as the purity level is defined. Likewise is OX3 directly dependent on the pressure in the reboiler for a specific purity level. With nitrogen purity of minimum 99% in NI1 and oxygen purity of minimum 95% in OX3 the pressure in the columns directly decides the temperatures.

A change in purity level will not have major impacts on the temperatures, but in a system with very small temperature differences it is important to be aware of the great sensitivity.

3.1.2.7 Subcooler

The nitrogen stream leaving the high pressure column needs to be cooled before entering the low pressure column. This is done in heat exchanger E3 and E4. They are not a part of the main heat exchanger and may be considered as a subcooler for the nitrogen stream. This is shown in figure 3.7.
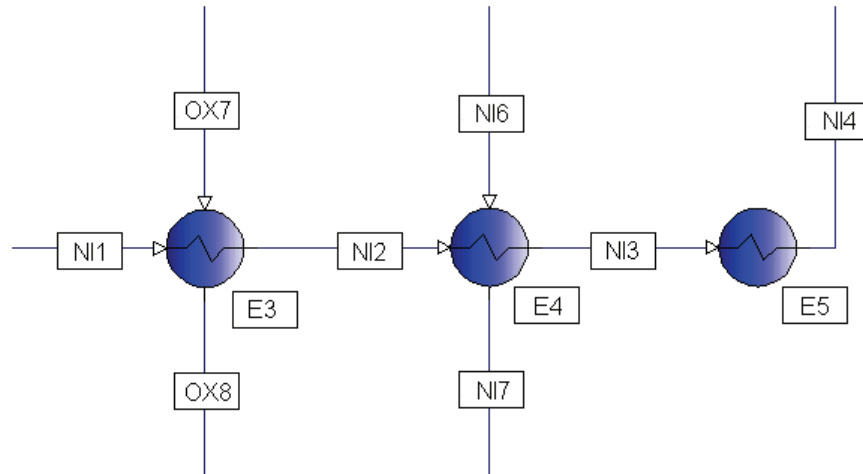
Figure 3.7. Model of subcooler.

Heat exchanger E5 is only included due to convergence in the model and has a neglectable duty.

3.1.2.8   After treatment of the air

In the original model there is no compression of either the nitrogen or oxygen stream out of the air separation island. This is since energy calculations of an ASU normally are done without oxygen compression and nitrogen often is considered as waste. To be able to compare the developed model with existing theory no after compression where originally made. An overview of the GOX plant is shown in figure 3.8.
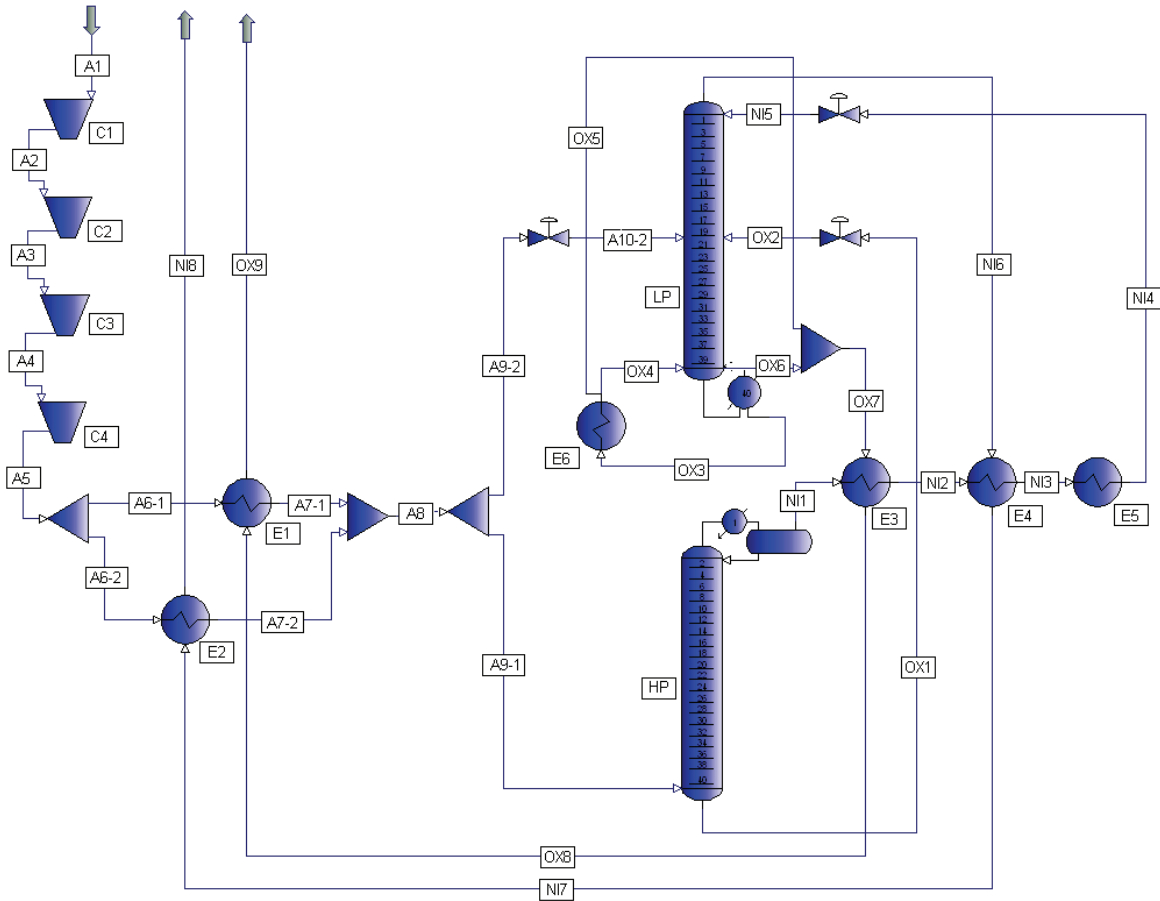
Figure 3.8. Model of GOX plant without oxygen compression.

To compare a GOX island with a LOX island the oxygen in both cases needs to be compressed to a wanted level. To compare the developed GOX and LOX models with each other and given literature, compressors are added on OX9.

In the final model used for energy considerations for a total power plant, compression of both the oxygen used for gasification and nitrogen used to dilute the fuel are compressed to a desirable level. The oxygen feed to the gasifier has a pressure level at 42bar and the fuel feed to the turbine has a pressure level at about 26bar.

3.1.3   Liquid oxygen

As mentioned in *2.1.2.10 Liquid oxygen* in theoretical background the oxygen compression in a LOX plant appears in liquid phase in stead of gaseous phase. Pumping liquid oxygen instead of compressing gaseous oxygen has safety advantages and may also lower the energy expenses. The LOX plant developed in PRO/II is based on the already explained GOX plant.

An overview of the LOX plant is given in figure 3.9.
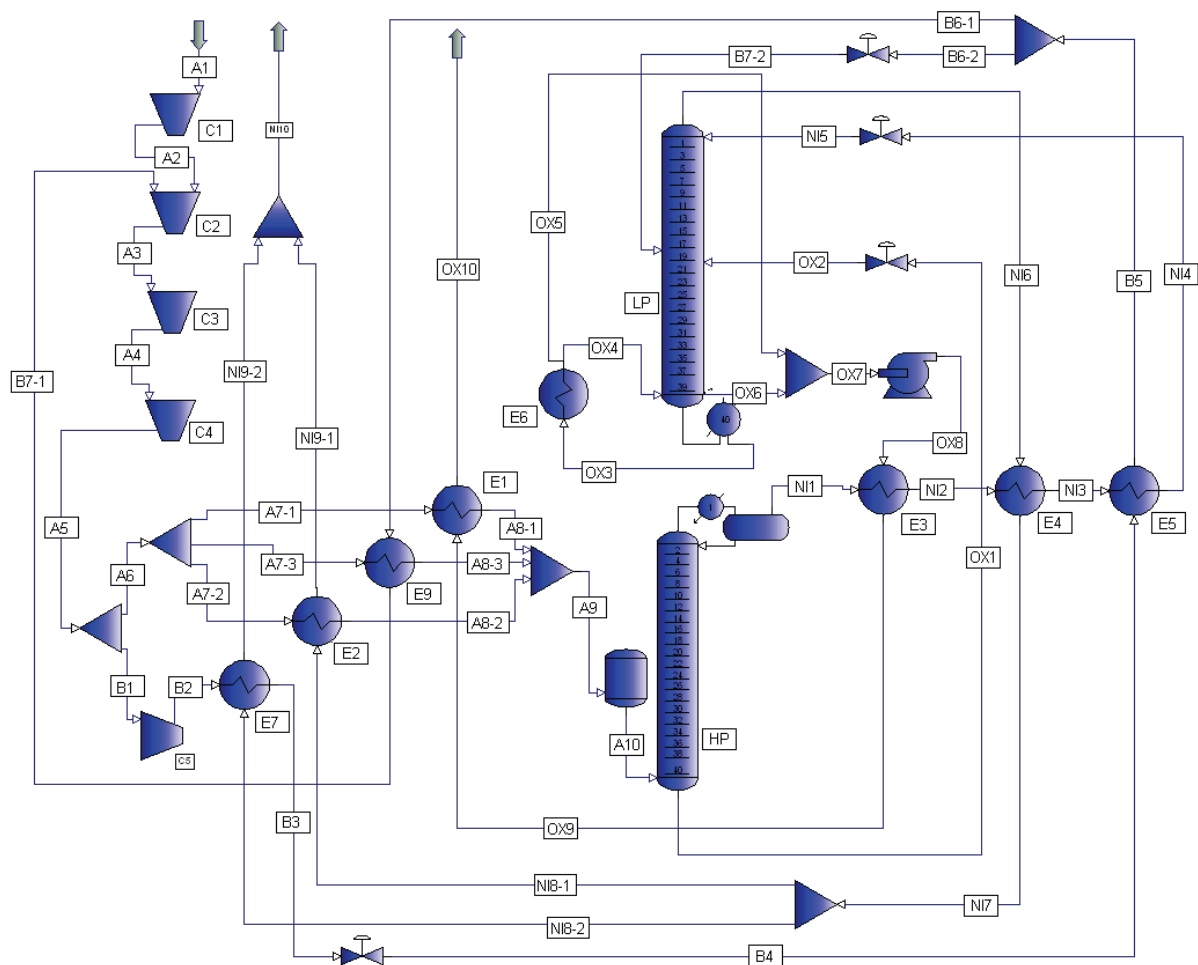
Figure 3.9. Model of a LOX plant.

3.1.3.1   Modifications compared to GOX model

The oxygen production of the plant is given by stream OX7 from the low pressure column. This stream is in liquid phase in both the GOX and LOX plant, but has in the GOX plant a change of phase through the heat exchanger cooling the nitrogen from the high pressure

column. At the entrance of E1 in the main heat exchanger the oxygen stream is in vapor phase.

In the LOX plant a pump is installed before the heat exchanging in E3 which causes phase change. Stream OX7 is therefore pumped to wanted pressure before entering heat exchanger E3. Because of the pressure rise there is no change of phase through heat exchanger E3. This leads to a very low heat exchanging in heat exchanger E3 and a subsequent need of cooling in the nitrogen stream between the high pressure and low pressure column. The oxygen stream entering the main heat exchanger in E1 is now in liquid phase and the phase change appears through this exchanger.

The need of cooling in the nitrogen stream between the high pressure and low pressure column must be covered by an internal made increase in heat removed from the island. This is done by installing a splitter after the main compressor and compress parts of the air further. The air is sent through heat exchanger E7, which is a part of the main heat exchanger, before it is choked to achieve more coldness. The coldness is then used to cool the nitrogen stream between the high pressure and low pressure column by heat exchanger E5.

3.1.3.2   Minimum temperature approach problems

As presented in the theoretical background the booster compressed air is choked to a pressure equal to high pressure column pressure. In the model developed for this report, it is not possible to cool the nitrogen stream with air at high pressure column pressure. If the air is choked to high pressure column level the temperature in the air is higher than the temperature in the nitrogen stream. This is shown in table 3.4.

Table 3.4. Stream properties for nitrogen from condenser and boosted air.

Stream Name			NI3	B4 – 6.00bar	B4 – 1.57bar
Phase			Mixed	Mixed	Mixed
Temperature	K		95.305	98.543	83.336
Pressure	bar		5.500	6.000	1.570
Flowrate	kmol/s		0.429	0.300	0.300
Composition					
O_2			0.005	0.210	0.210
N_2			0.990	0.781	0.781
AR			0.005	0.009	0.009

Air in mixed phase at 6bar, *B4 – 6.0bar*, has a higher temperature than the nitrogen that need to be cooled, NI3. One solution is to cool air at 6bar to a temperature which makes it possible to heat exchange with NI3. Because air is in mixed phase and has its critical temperature at 98.543K at 6bar, this would demand an unacceptable energy amount. To be able to cool NI3 the air needs to be choked further, to a pressure level lower than the high pressure column.

If the air is choked lower than the pressure level in the high pressure column it can not be fed directly to the high pressure column. The solution for this is to feed parts of the air to the low pressure column and recompress the rest. The recompression may either be done by an extra compressor, by mixing the low pressured air stream with booster compressed air to a suitable pressure level, or by feeding the air back to the main compressor. The most energy efficient solution is to feed the low pressured air back to the main compressor. Without need of extra compressors this is also a less maintenance demanding.

At what pressure B4 should be choked to is dependent on the energy amount that needs to be exchanged with NI3 and how the pressure should be increased again afterwards. Because of the energy that need to be exchanged between NI3 and B4 it was found out that the pressure had to be equal to or below 2bar. To match one of the steps in the main air compressor for recompression the pressure is set to 1.57bar, see table 3.2 and 3.3. Stream properties of boosted air is shown as *B4 – 1.5bar* in table 3.4.

In the GOX model, heat exchanger E5 is independent and included for the model to converge. Heat exchanger E5 is in the LOX model integrated and the duty is covered internally. The flash tank before the high pressure column is therefore included to have an independent unit "helping" the model converge. The purpose of the flash tank is to set the temperature of the outgoing air stream to dew point. This flash tank may be seen as a heat exchanger setting the temperature of the stream to dew point. The air stream entering the flash tank is very near dew point and the duty of the tank is neglectable. It is possible to run the model without the flash tank, but even minor input changes then leads to convergence problems.

3.1.4   *Argon treatment*

Argon removal is not handled in the developed models. The slightly raised purity level in the oxygen and nitrogen achieved by removal of argon has no major improvements on either the Gasification Island or the Power Island. To justify implementation of an argon column in an ASU for IGCC purpose, the argon captured has to be sold at an acceptable price. This report does not focus on economic profits by operating in the argon market and the additional column is therefore not implemented.

3.2   Gasification Island

3.2.1   *Simulation tools*

The Gasification Island is also simulated in PRO/II 8.0.

PRO/II is normally used for fluids and the first approach is to verify if the program could handle solid fuels like coal. There are run simulations on a self made coal composition and on a structure where coal is defined as a gas. The testing of PRO/II was a part of the project work during autumn 2007. A short repetition of this work is presented here. Thereafter modeling of different coal types is presented.

There are also done calculations in MatLab version R2007a. The calculations performed are equilibrium calculations on the gasification procedure. This is done to solve a gasification problem from simple formation reactions to finished syngas composition.

In addition to MatLab and PRO/II, an online chemical equilibrium calculator is used [26]. This tool is utilized to check the validity of simulations and calculations performed.

3.2.2   *MatLab calculations*

The formation reactions are the heart of the gasifier. From the formation reactions together with mass balances, a set of equations giving the syngas composition may be derived. To solve such a complex equation set the mathematical computer tool MatLab is used. Calculating a syngas composition in MatLab demands manually equation derivation. MatLab is only an equation solver and the derivation from formation reaction to a solvable equation set is done manually. The reason for doing this is to show that the results calculated from simple formation reactions corresponds to calculated values from more advanced computer tools as PRO/II and the chemical equilibrium calculator.

3.2.2.1 Complete equation set

From the formation reactions presented in the theoretical background it is possible to calculate the syngas composition. The conversion of coal, oxygen and steam to syngas is decided by these formation reactions together with input values as temperature, pressure and coal composition. The coal composition is assumed to be a combination of C, H, O, N and S. The seven independent formation reactions are presented in *2.2.2.1 Formation reactions* and are repeated below.

$C + 1/2\,O_2 \rightleftarrows CO$	-111 MJ/kmol	(2.30)
$C + O_2 \rightarrow CO_2$	-394 MJ/kmol	(2.31)
$C + 2H_2 \rightleftarrows CH_4$	-75 MJ/kmol	(2.33)
$H_2 + 1/2\,O_2 \rightleftarrows H_2O$	-242 MJ/kmol	(2.35)
$1/2\,N_2 + 1/2\,O_2 \rightleftarrows NO$	+90 MJ/kmol	(2.36)
$S + O_2 \rightleftarrows SO_2$	-362 MJ/kmol	(2.37)
$S + H_2 \rightleftarrows H_2S$	-85 MJ/kmol	(2.38)
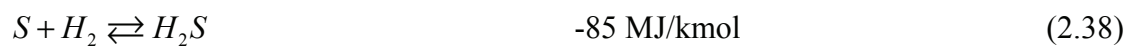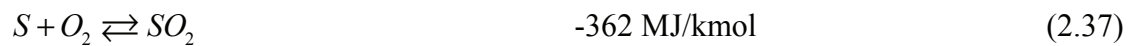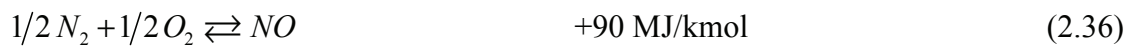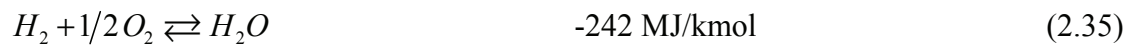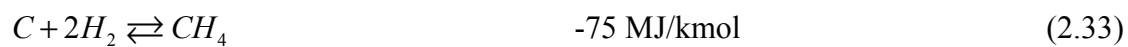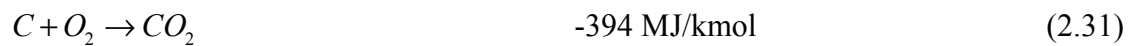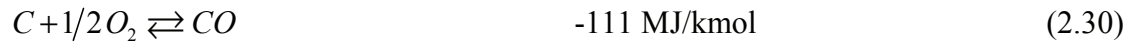
The reactions contain a total of 12 substances. In theory traces of all 12 substances is found in the syngas composition and the equation set therefore contains a minimum of 12 unknown. In calculations it is not necessary to include all 12 substances in the equilibrium. This is due to neglectable amount of several of the substances. A method containing all 12 substances is although presented before the set of equations is reduced to containing only the relevant ones.

All the reactions have belonging equilibrium equations presented in chapter *2.2.2.2 Equilibrium equations*. The equilibrium equations are derived from the formation reactions and the deriving procedure is described in Appendix A. The equilibrium equations are repeated below.

$$K_{CO} = \frac{[y_{CO}]}{[y_C][y_{O_2}]^{\frac{1}{2}} p^{\frac{1}{2}}} \qquad (2.40)$$

$$K_{CO_2} = \frac{[y_{CO_2}]}{[y_C][y_{O_2}] p} \qquad (2.41)$$

$$K_{H_2O} = \frac{\left[y_{H_2O}\right]}{\left[y_{H_2}\right]\left[y_{O_2}\right]p^{\frac{1}{2}}} \tag{2.42}$$

$$K_{CH_4} = \frac{\left[y_{CH_4}\right]}{\left[y_C\right]\left[y_{H_2}\right]^2 p^2} \tag{2.43}$$

$$K_{NO} = \frac{\left[y_{NO}\right]}{\left[y_{O_2}\right]^{\frac{1}{2}}\left[y_{N_2}\right]^{\frac{1}{2}}} \tag{2.44}$$

$$K_{SO_2} = \frac{\left[y_{SO_2}\right]}{\left[y_S\right]\left[y_{O_2}\right]p} \tag{2.45}$$

$$K_{H_2S} = \frac{\left[y_{H_2S}\right]}{\left[y_S\right]\left[y_{H_2}\right]p} \tag{2.46}$$

The 12 unknown molar fractions are implemented in equation 2.40 to 2.46. Equation 2.40 to 2.46 are also the first 7 equations in the equation set. The equilibrium constants K are tabulated for given temperatures.

The element mass balances for the five feed substances are independent equations and are implemented in the equation set. An element mass balance equation gives that the amount of an element fed to a process must equal the amount of the element going out of the process. If 1kmol/s of C is fed to the gasifier the sum of C, CO, CO_2 and CH_4 also must equal to 1kmol/s. In this process there are five elements in the feed giving five element mass balances.

$$y_{C_{Feed}} = (y_C + y_{CO} + y_{CO_2} + y_{CH_4})n \tag{3.1}$$

$$y_{H_{Feed}} = (4y_{CH_4} + 2y_{H_2} + 2y_{H_2O} + 2y_{H_2S})n \tag{3.2}$$

$$y_{O_{Feed}} = (y_{CO} + 2y_{CO_2} + 2y_{O_2} + 0.5y_{H_2O} + y_{NO} + 2y_{SO_2})n \tag{3.3}$$

$$y_{N_{Feed}} = (2y_{N_2} + y_{NO})n \tag{3.4}$$

$$y_{S_{Feed}} = (y_S + y_{SO_2} + y_{H_2S})n \tag{3.5}$$

C, N and S are in theory fed to the gasifier process only through the coal. H and O are fed both through the coal and through the feeds of oxygen and steam. When calculating the element feeds it is therefore important to include the H and O feed from steam and oxygen in

addition to the feed from the coal. If the calculation should be extremely precise the few percent of nitrogen in the oxygen feed from the ASU and possible pollution in the water also needs to be taken into account.

The equation set now contains 12 equations, but the introduction of the variable giving the total number of moles in the equilibrium gas mixture, n, makes need for an extra equation. This is solved by the equation of the total mass balance.

$$y_C + y_{CO} + y_{CO_2} + y_{CH_4} + y_{O_2} + y_{H_2} + y_{H_2O} + y_{N_2} + y_{NO} + y_S + y_{SO_2} + y_{H_2S} = 1 \qquad (3.6)$$

The equation set now contains 13 equations with 13 unknown.

3.2.2.2 Reduction of the equation set

The equation set containing 13 equations and 13 unknown is very complex to solve. In fact, the extremely small amount of some of the substances makes a MatLab model not able to solve the equation set. When the molar fractions get this close to zero and other mole fractions are divided by these the model is unsolvable. The solution is to reduce the set of equations to a set containing only the substances with practical influence of the syngas composition.

The amount of CH_4, NO, H_2S and SO_2 are considered to small to have major impact on the syngas composition. The remaining independent formation reactions are then 2.30, 2.31 and 2.35.

$$C + 1/2 O_2 \rightleftarrows CO \qquad (2.30)$$
$$C + O_2 \rightarrow CO_2 \qquad (2.31)$$
$$H_2 + 1/2 O_2 \rightleftarrows H_2O \qquad (2.35)$$
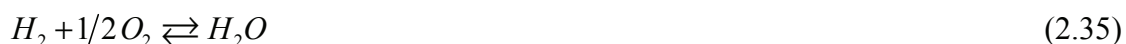
This assumption also gives that there is no nitrogen or sulfur in the coal composition. This is a simplification need to be done to get the MatLab model to converge. The coal is then containing of a combination of carbon, hydrogen and oxygen.

It is also assumed that all the oxygen is consumed in the gasification process and there is no oxygen left in the syngas. This reduces the three independent formation reactions to two new formation reactions. These reactions are independent of each other, but are dependent of the previous three.

The first new formation reaction, 2.32, is derived by subtracting 2.31 from 2.30 multiplied with two.

$$C + CO_2 \rightleftarrows 2CO \tag{2.32}$$

The other new formation reaction, 2.24, is derived by subtracting 2.35 from 2.30.

$$C + H_2O \rightleftarrows CO + H_2 \tag{2.34}$$

It is further assumed that all the carbon is gasified and there is no pure carbon left in the syngas. In real life some of the carbon is not gasified and leaves the gasifier together with ash and slag. It is although a legal approximation assuming no carbon in the syngas.

Subtraction of 2.34 from 2.32 gives a formation reaction without pure carbon.

$$CO + H_2O \rightleftarrows CO_2 + H_2 \tag{3.10}$$

From 3.10 the following equilibrium constant can be set up.

$$K = \frac{[y_{CO_2}][y_{H_2}]}{[y_{CO}][y_{H_2O}]} \tag{3.11}$$

Equation 3.11 contains five unknown. First of all the K value is derived.

$$C + 1/2\,O_2 \rightleftarrows CO \Rightarrow K_{CO} = \frac{[y_{CO}]}{[y_C][y_{O_2}]^{\frac{1}{2}}p^{\frac{1}{2}}} \Rightarrow [y_{CO}] = K_{CO}[y_C][y_{O_2}]^{\frac{1}{2}}p^{\frac{1}{2}} \tag{3.12}$$

$$C + O_2 \rightarrow CO_2 \Rightarrow K_{CO_2} = \frac{\left[y_{CO_2}\right]}{\left[y_C\right]\left[y_{O_2}\right]p} \Rightarrow \left[y_{CO_2}\right] = K_{CO_2}\left[y_C\right]\left[y_{O_2}\right]p \qquad (3.13)$$

$$H_2 + 1/2\,O_2 \rightleftarrows H_2O \Rightarrow K_{H_2O} = \frac{\left[y_{H_2O}\right]}{\left[y_{H_2}\right]\left[y_{O_2}\right]p^{\frac{1}{2}}} \Rightarrow \left[y_{H_2O}\right] = K_{H_2O}\left[y_{H_2}\right]\left[y_{O_2}\right]p^{\frac{1}{2}} \quad (3.14)$$

The K value is found by inserting 3.12, 3.13 and 3.14 in 3.11.

$$K = \frac{\left[y_{CO_2}\right]\left[y_{H_2}\right]}{\left[y_{CO}\right]\left[y_{H_2O}\right]} = \frac{K_{CO_2}\left[y_C\right]\left[y_{O_2}\right]p\,\left[y_{H_2}\right]}{K_{CO}\left[y_C\right]\left[y_{O_2}\right]^{\frac{1}{2}}p^{\frac{1}{2}}K_{H_2O}\left[y_{H_2}\right]\left[y_{O_2}\right]p^{\frac{1}{2}}} = \frac{K_{CO_2}}{K_{CO}\bullet K_{H_2O}} \qquad (3.15)$$

This gives an equation with four unknown.

$$\frac{K_{CO_2}}{K_{CO}\bullet K_{H_2O}} = \frac{\left[y_{CO_2}\right]\left[y_{H_2}\right]}{\left[y_{CO}\right]\left[y_{H_2O}\right]} \qquad (3.16)$$

K_{CO2}, K_{CO} and K_{H2O} are tabulated for specific temperatures. In some literature the equilibrium constant in equation 3.11 are tabulated directly and the derivations performed in 3.12 to 3.16 are not necessary. It is although shown here to give the entire derivation from the elementary formation reaction to the calculated syngas composition.

The next three equations are given by element mass balance and form a new unknown, n.

$$y_{C_{Feed}} = (y_{CO} + y_{CO_2})n \qquad (3.17)$$

$$y_{H_{Feed}} = (2y_{H_2} + 2y_{H_2O})n \qquad (3.18)$$

$$y_{O_{Feed}} = (y_{CO} + 2y_{CO_2} + 0.5y_{H_2O})n \qquad (3.19)$$

Here is $y_{C,Feed}$ the number of moles of carbon in the coal. $y_{H,Feed}$ is moles of hydrogen in the coal plus the moles of steam multiplied with two. The addition of two times the number of moles of steam is to add on the two hydrogen atoms in H_2O. Equally $y_{O,Feed}$ is moles of

oxygen in the coal plus to times the number of moles of O_2 plus the number of moles of steam.

The last equation which completes the equation set and is the total mass balance.

$$y_{CO} + y_{CO_2} + y_{H_2} + y_{H_2O} = 1 \tag{3.20}$$

The equation set then consists of five equations with five unknown. This is a set of equations solvable in MatLab and a script using the fsolve function is made.

The script with the function to solve the five equations is given in Appendix B. The script which runs the function is given in Appendix C. Results from the calculations are presented and compared with results from other computer tools in the discussion part of the report.

3.2.3   PRO/II testing

In this part the validity of PRO/II are tested. The goal is to prove that PRO/II could handle solid fuels. PRO/II is normally used in models containing fluids.

The first challenge is to create a gasification island that produced syngas. The purpose of the gasifier is to convert coal, water and oxygen into useful gasses. Syngas is mainly a mix of carbon monoxide and hydrogen. Both CO and H_2 have heating value. They can react with oxygen and release energy. Because of the CO_2 removal, the goal for this model is to maximize the hydrogen production and remove the carbon before the gas turbine cycle. Figure 3.10 shows a gasification island that involves a gasifier and a shift reactor. The syngas cooler between the gasifier and the shift reactor reduces the temperature before the water shift reaction to maximize the production of H_2. The heat extracted from this heat exchanging can be used in the steam cycle. This will be discussed later when a complete plant is described.
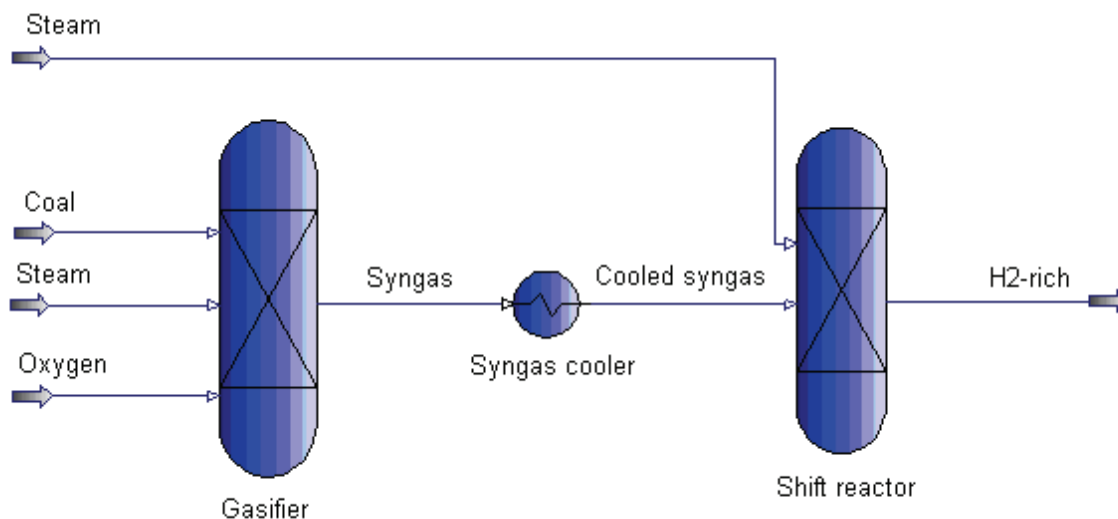
Figure 3.10. Gasification Island.

Figure 3.10 gives an overview of the gasification process. Coal enters the gasifier and reacts with oxygen and steam to produce syngas. The syngas is cooled and fed into the shift reactor to enhance the hydrogen content.

3.2.3.1   Coal composition

PRO/II is a simulation tool that normally operates with fluids and not solids. Building a realistic coal structure in PRO/II is not straightforward. Coal is a large structure with a lot of chemical bindings between the different elements.

Coal is mainly containing carbon, hydrogen, oxygen, nitrogen and sulfur. The contents are bound in different ways and appear as a solid. Because PRO/II not handles coal as one single component, there is built a structure on an element basis. H, O and N as elements only occur in structures. If they are "released" they form molecules as H_2, O_2 and N_2. Under normal circumstances these substances are in gaseous phase, which also is the case in PRO/II. C and S are although possible to define as solids in PRO/II. S can also be defined as a gaseous substance. The coal fed to the gasifier is therefore a mixture of solid C and gaseous S, H_2, O_2 and N_2.

3.2.3.2 Coal defined as a chosen composition

In the first simulations there it is made a relative random assumption about the coal composition. This composition is shown in table 3.1.From the molar composition the mass composition is calculated. For this composition H_2, O_2 and N_2 is as mentioned defined as gases. This is a source to deviation compared to gasification with real life coal, but it is considered as an acceptable approximation.

Table 3.5. Molar and mass fractions.

Substance	C	H_2	O_2	N_2	S
Molar weight	12,00	2.016	32,00	28,00	32.06
Molar fraction	0.70	0.10	0.10	0.05	0.05
Mass fraction	0.5674	0.0136	0.2160	0.0948	0.1082

The total molar weight for a mixture is calculated from equation 3.21.

$$M_{coal} = \sum_{i=1}^{j} y_i M_i \qquad (3.21)$$

Where y_i is the molar fraction and M_i is the molar weight for the given substance. For the coal composition in table 3.5 the molar weight becomes 14.82kg/kmol.

This model is only used to test if the program handles solids fed to a gasifier. It had to be checked what reactions occurred and if the simulated gasification process looked realistic.

A simulation of the composition containing fixed carbon, optimized for maximal CO production in the gasifier and 98% of the CO is converted in the water gas shift reaction, gave the results given in table 3.6.

Table 3.6. Gasification of coal containing fixed carbon.

	Coal	Oxygen	Water to gasifier	Syngas	Water to shift	H_2 rich gas
Temperature	15.000	15.000	300.000	1787.728	180.000	20.000
Pressure	8.000	8.000	8.000	7.900	7.900	7.900
Flowrate	1.000	0.285	0.255	1.201	0.548	1.749
Composition						
C	0.700	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.000	0.000	0.576	0.000	0.011
CO_2	0.000	0.000	0.000	0.007	0.000	0.389
O_2	0.100	1.000	0.000	0.039	0.000	0.027
H_2	0.100	0.000	0.000	0.192	0.000	0.516
H_2O	0.000	0.000	1.000	0.103	1.000	0.000
CH_4	0.000	0.000	0.000	0.000	0.000	0.000
N_2	0.050	0.000	0.000	0.042	0.000	0.029
NO	0.000	0.000	0.000	0.000	0.000	0.000
S	0.050	0.000	0.000	0.000	0.000	0.000
SO_2	0.000	0.000	0.000	0.042	0.000	0.029
H_2S	0.000	0.000	0.000	0.000	0.000	0.000

To be able to verify this simulation as realistic, a similar simulation where coal is defined as a gaseous substitute must be performed.

3.2.3.3 Coal defined as a composition of CO, CO_2 and CH_4

Because PRO/II is designed to operate with fluids it has to be performed a test on the validity of calculations containing solids.

To verify this coal is defined as a gaseous mixture of CO, CO_2 and CH_4. In this definition the heating value of the pure carbon together with N_2, H_2, O_2 and S do not equal the heating value of the combination of CO, CO_2 and CH_4. This calculation leaves out the energy balance and looks specific into the molar balance. The amount of the different atoms, C, H, O, N and S, has to be the same in the two cases. If there is a surplus or a shortage of a substance this has to be regulated by the use of steam and oxygen in the gasifier. Amore detailed procedure of the comparison is presented in Appendix D.

It should be noted that temperatures and pressures in the test model is not valid for further simulations. The syngas temperature of 1788˚C is too high for a gasifying process, and the pressure is normally higher. In section *3.2.4 PRO/II simulations* a more realistic coal composition is presented and the temperatures and pressures will get values closer to real life.

To compare the solid carbon model with a coal as gas model, it is made a composition that on molar basis is equal to the fixed carbon composition. The coal as gas model contains considerable amounts of oxygen due to the CO and CO_2 substances. This brought along an oxygen surplus compared to the fixed carbon model and this is adjusted in the oxygen feed. Due to this difference, the oxygen feed was set to 0.100 instead of 0.285. The model has fixed temperature and pressure levels equal to the fixed carbon simulation. This is done since the heating value is different in the two simulations. To be able to compare the outcomes the operational conditions must although be equal. Gasification temperature is in the simulation with coal defined as gases therefore fixed and equal to the previous simulation. The results are presented in table 3.7.

Table 3.7. Gaseous substitute with fixed O_2 and H_2O amounts.

	Coal as gas	Oxygen	Water to gasifier	Syngas	Water to shift	H2 rich gas
Temperature	15.000	15.000	300.000	1787.728	180.000	20.000
Pressure	8.000	8.000	8.000	7.900	7.900	7.900
Flowrate	0.800	0.100	0.255	1.201	0.548	1.749
Composition						
C	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.688	0.000	0.000	0.576	0.000	0.011
CO$_2$	0.125	0.000	0.000	0.007	0.000	0.389
O$_2$	0.000	1.000	0.000	0.039	0.000	0.027
H$_2$	0.000	0.000	0.000	0.192	0.000	0.516
H$_2$O	0.000	0.000	1.000	0.103	1.000	0.000
CH$_4$	0.063	0.000	0.000	0.000	0.000	0.000
N$_2$	0.063	0.000	0.000	0.042	0.000	0.029
NO	0.000	0.000	0.000	0.000	0.000	0.000
S	0.063	0.000	0.000	0.000	0.000	0.000
SO$_2$	0.000	0.000	0.000	0.042	0.000	0.029
H$_2$S	0.000	0.000	0.000	0.000	0.000	0.000

This simulation returned the exact same composition as the simulation fed with fixed carbon. As long as the temperature in the gasifier and the total feed of moles of C, H, O, N and S is equal it was unessential if the coal is fed as fixed carbon or a combination of gaseous substitutes. This is as mentioned only a molar analysis. The energy balance will not be correct when the coal is defined different than realistic coal.

It can therefore be concluded that PRO/II handles gasification of fixed carbon on a molar basis. PRO/II may therefore be used in gasification simulations.

3.2.4   *PRO/II simulations*

The validity of PRO/II is proved and simulations on realistic coals are now performed.

The production of syngas involves reaction between the feedstock, oxygen and/or steam. The amount of O_2 and steam affect the process directly. A basic rule is more O_2 gives higher temperature and more steam lowers the temperature. For IGCC applications the oxygen consumption is one of the major input factors. The air separation unit presented in *3.1 Air Separation Island* delivers the needed oxygen amount to the Gasification Island.

3.2.4.1   Introduction

Type of gasifier and coal type is directly affecting the gasification process regarding to consumption of oxygen and steam, produced syngas, pressure and operation temperature. Table 2.5 and 2.6 in *2.2.3.3 Entrained-flow gasifiers* gives an overview of the composition in the product gas and the steam/oxygen consumption. In addition, it gives the amount of syngas produced per ton coal. Three of the coals will be studied closer here; the Browncoal from Rhein, the Bituminous from Datung and the Anthracite from Ruhr. These coals are ranked on different levels and will behave different in a gasification process. This chapter describes how these models are developed. The main emphasis is placed on the oxygen (and steam) consumption.

Table 3.8 gives an ultimate analysis of the three coals. It does not include the trace elements generalized as ash. These are typical SiO_2, Al_2O_3, Fe_2O_3 among others. Ash is generally considered as being inert in the calculations. The main difference for these coals is the carbon content. The Anthracite from Ruhr has a high carbon fraction and therefore a higher heating value and a higher rank.

Table 3.8. Tabulated mass fraction for given coals.

Coal		Mass Fraction				
Region	Classification	C	H	O	N	S
Rhein	Browncoal	0.675	0.05	0.265	0.005	0.005
Datung	Bituminous	0.844	0.044	0.095	0.009	0.008
Ruhr	Anthracite	0.918	0.036	0.025	0.014	0.007

It should be noted that table 3.8 gives the composition based on a maf ultimate analysis. Coal often contains a lot of water and it is not efficient to first remove that and thereafter add steam in the gasifier. The Browncoal is typical a coal containing a lot of water. This will be studied closer in the next chapter. The other coals will be handled as dry coal, where steam supply is required to get the wanted gasification process.

Having the mass fraction for the different coals the molar fraction can be calculated. This is done because the modeling procedure in PRO/II uses molar fractions. The method of converting from mass fraction to molar fraction is shown for H_2 in equation 3.22.

$$y_{H_2} = \frac{\dfrac{m_{H_2}}{M_{H_2}}}{\sum\limits_{i=1}^{j} \dfrac{m_i}{M_i}} \qquad\qquad (3.22)$$

Where m is the known mass fraction and M is the molar weight. This method is usable for all substances. Using Excel or MatLab the converting process is straightforward and shown in table 3.9.

Table 3.9. Calculated molar fraction for given coals.

Coal		Mol Fraction				
Region	Classification	C	H_2	O_2	N_2	S
Rhein	Browncoal	0.623	0.278	0.093	0.002	0.000
Datung	Bituminous	0.735	0.228	0.031	0.003	0.003
Ruhr	Anthracite	0.798	0.186	0.008	0.005	0.002

The literature gives an overview for expected product gases for given coals [6]. Table 3.10 shows a dry gas analysis for the coals using an Entrained-Flow Gasifier. The A indicates the amount of unburned ash. This is a review of the tables presented in chapter *2.2.3.3 Entrained flow gasifier*, but here is only for the chosen coal types shown.

Table 3.10. Expected product gas for given coals [6].

Coal		Product Gas Mol Fraction (dry)					
Region	Classification	CO	H_2	CO_2	N_2	A	H_2S
Rhein	Browncoal	0.61	0.29	0.08	0.01	0.01	0.002
Datung	Bituminous	0.66	0.31	0.01	0.01	0.01	0.002
Ruhr	Anthracite	0.65	0.31	0.01	0.01	0.01	0.002

Table 3.10 indicates that the product gas does not vary considerable due to different feedstock. The main differences are easier observed comparing with table 3.11. This table gives an overview of the expected amount of syngas for a given mass for a specific coal. In addition it shows the consumption of steam and oxygen.

Table 3.11. Steam/oxygen consumption for given coals [6].

Coal		Amount of reactants and products		
Region	Classification	Nm^3 syngas/ ton maf coal	Nm^3 O_2/ Nm^3 syngas	kg steam/ Nm^3 syngas
Rhein	Browncoal	965	0.33	0
Datung	Bituminous	2060	0.27	0.09
Ruhr	Anthracite	2270	0.26	0.13

Table 3.11 shows the consumption of O_2 and steam from the gasification process for the three different coals. In the case of IGCC with CO_2 capture more steam is required in the shift reformer to maximize hydrogen production. The amount of additional steam in the water gas shift reformer depends on the water content in the syngas, wanted output composition etc. According to literature the molar rate of H_2O over CO is normally in the area 1.4 - 2.0 [21]. This will be discussed closer in *4.2.5.1 Water gas shift reactor*.

3.2.4.2   Modeling Gasification Islands

Figure 3.10 shows a model of the gasification process including a shift reactor. This is the main processes in the Gasification Island. The wanted rate of oxygen and steam is assumed covered and the feed amount is unlimited. When the Gasification Island is itegrated with the other islands the need of oxygen and steam is covered by the ASU and Power Island respectively.

For IGCC applications entrained-flow gasifiers are the most common facility to use. In the following part three gasification processes is studied closer. Three models are shown and modeled in PRO/II. One of them is a typical Coal-Water Slurry-Fed Gasifier and the two others are Dry-Coal Feed gasifiers. It should be noted that these models are simplified to fit in the PRO/II modeling program. The calculation tool is not made for handling coal feeds using slurry Pumps and lock hoppers. Anyway the sheet will show the main principles around the gasification process. The models are made to fit real life processes regarding to temperature,

pressure, consumption of oxygen/steam and production rate. The basis of the Gasification Island is presented in figure 3.11.
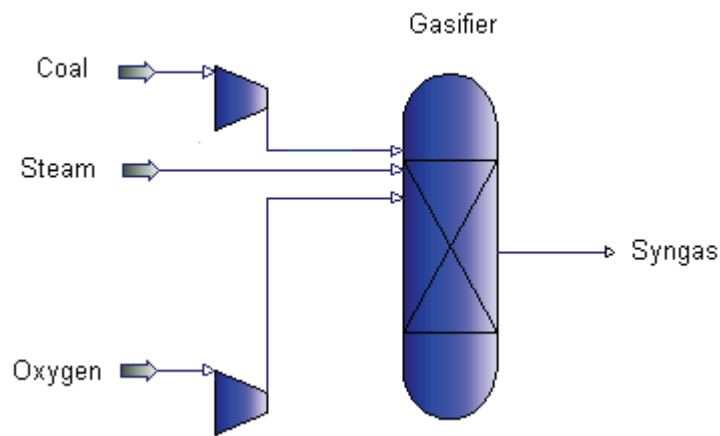
Figure 3.11. Model of a gasifier.

Figure 3.11 shows the main principles of a dry fed Gasification Island. Modifications are made to fit the slurry feed gasifier, which in the model means to remove the steam supply. This type will be discussed in the upcoming part followed by two examples of Dry-Coal Feed gasifiers.

The goal for these models are to build gasification islands that gives realistic composition of syngas using expected input amounts of O_2 and H_2O. The required amount of oxygen and steam are interesting because they must be covered internally and this affects the total plant efficiency.

Table 3.11 gives the values on normal cubic meter (Nm^3). The chemical report in PRO/II operates with standard cubic meters (Sm^3) for gasses. Nm^3 is defined as the gas volume at a pressure of 1.101325 bar and a temperature of 15˚C. In PRO/II, Nm^3 is achieved by installing a heat exchanger with the given conditions in the product stream. This is shown in figure 3.12.
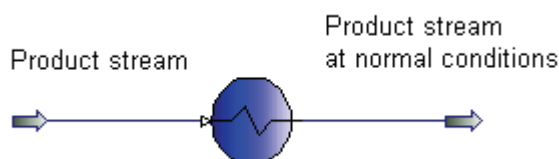
Figure 3.12. Product stream at normal conditions.

Alternatively, the standard state results from the chemical report could be multiplied with a correction factor. This factor is about 1.055. The models in PRO/II use mol as the unit to measure the amounts of the different matters. The conversion to Nm^3 etc. is done to fit the values from the literature. The values from the literature are mainly found in *Gasification* by Higman and van der Burgt [6]. The values are empirical numbers found from existing plants. Comparing the simulation results with these numbers will give a relevant check according to syngas composition and O_2/steam consumption.

Gasification of Browncoal

The Browncoal from Rhein contains a relatively high amount of water. This justifies table 3.11 that suggests no steam consumption in the gasification process. Browncoal is actually not a good coal for gasification. It is a coal with high moisture content and requires more oxygen than higher ranked coals per produced unit of syngas. However, the high content of water makes this coal type useful for Coal-Water Slurry-Fed Gasifiers. A gasification model with Browncoal is therefore made to simulate a gasifier like this. Figure 3.13 shows a model of a slurry-fed gasifier. The steam is in this model fed as water content in the coal. The figure also shows a water gas shift reactor. This will be explained further in *3.2.6 Water shift reforming*.

The model is a simplification of a real slurry-fed. In these units the coal is compressed using an advanced pump, while in this model a simple compressor is used for the pressure rise. The inlet pressure is set to 42bar for both the oxygen and the coal slurry. The pressure loss in the gasifier is set to 0.4bar. For a slurry feed the pressure may be even higher. This is however considered as unnecessary since the products in this case are supposed to be used in a power plant. In a power plant the turbine inlet pressure is normally about 15-35bar [16]. The reason for choosing a pressure of 42bar is to increase the capacity without increasing the equipment size. A high pressure is also favourable regarding to CO_2 capture.
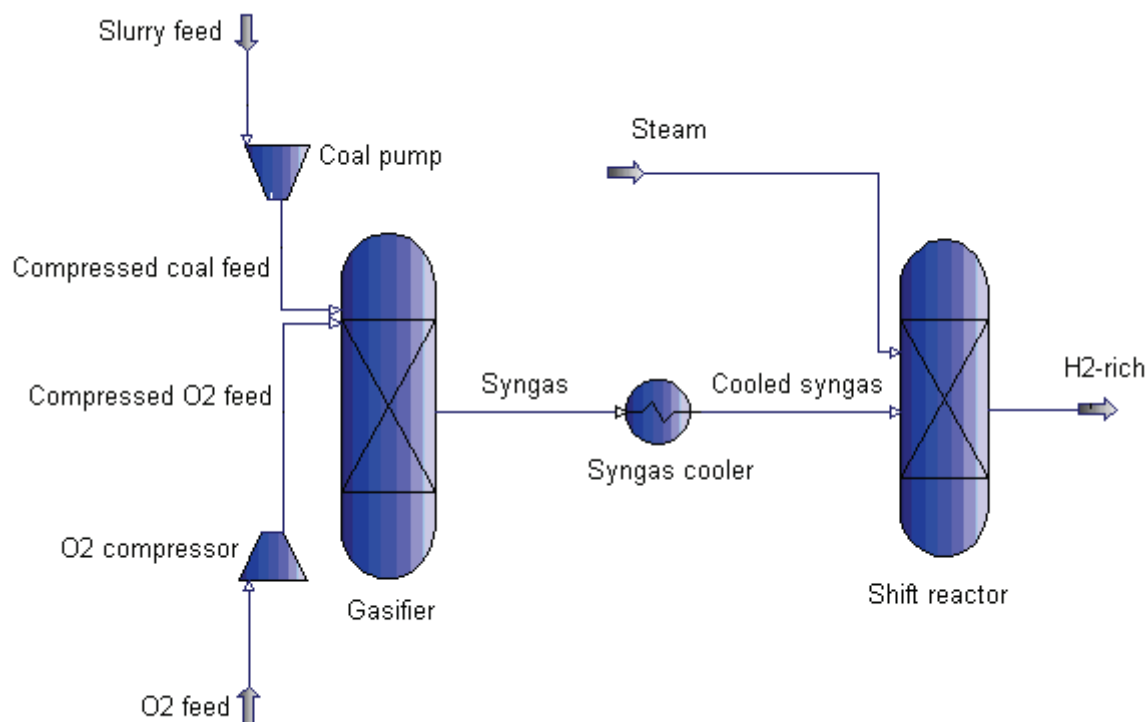
Figure 3.13. Model of slurry feed gasifier.

Browncoal may contain considerable amounts of water. A proximate analysis on mass as received (ar) basis may give up to 60% water [6]. The starting point for calculations on the Browncoal is the ultimate analysis from table 3.8. This is transformed to molar fraction for PRO/II use in table 3.9. The coal is presented as maf, so water is added to the composition to make a model of slurry coal. There are done calculations on different amounts of water content in the coal. The water amount in the coal and the oxygen supply are adjusted to reach satisfactory temperatures, gasification products and consumption rates. Table 3.12 gives the final compositions when water is included in the Browncoal.

Table 3.12. Final composition.

Substance	C	H_2	O_2	N_2	S	H_2O
Molar weight	12.010	2.016	32.000	28.010	32.060	18.020
Molar fraction	0.487	0.215	0.071	0.002	0.002	0.223
Mass fraction	0.461	0.034	0.179	0.004	0.005	0.317

For this model the water percentage is 31.7%. Coal may have higher water content than this. If the level of moist is too high, drying should be done before the gasification process. The

drying process should occur naturally without external energy supply, for example by using air.

The calculations around the gasification of Browncoal is shown and discussed in *4.2.3.1 Gasification of Browncoal*.

Calculations on oxygen and steam consumption for Bituminous and Anthracite

Bituminous and Anthracite are high ranked coals which are suitable for gasification. The oxygen consumption is relatively low. Typical values for this is presented in table 3.11.

A gasification model like the one shown in figure 3.11 is built to gasify coal types similar to Bituminous and Anthracite, given in table 3.8 and 3.9. In this model the amount of coal and the gasification pressure is defined as constant. 1kmol of coal is pressurized and fed to the gasifier with a gasification pressure at 42bar. Pressurizing of coal is described in *2.2.3.5 Feeding procedures for a gasifier*. In the model the feeding procedure is modeled as a compressor. When the overall energy balance of a whole IGCC is calculated, there is added an adjusted work for the feeding procedure. From literature the energy consumption for this is suggested to be 11 MJ for 100 kg maf coal intake [6]. This is included in the overall calculation in *4.5.1 Initial calculations*.

The oxygen and steam are used as variables to reach a satisfactory composition of syngas. In addition the gasification temperature must not exceed possible level for these facilities. A rule of thumb says that more oxygen increases the temperature and more steam reduces the temperature.

To make a relevant comparison, the production rate, the oxygen/steam consumption, the syngas composition and the gasification temperature should not vary too much from the values in table 3.10 and 3.11**.** These values are calculated doing iteration between the input factors.

The first step is to find a production rate, which means amount of Nm^3 syngas per ton of maf coal. This number is expected to vary from the literature since the gasification model deals with coal as a composition of five elements and not a complete material. A heat exchanger is,

similar to figure 3.12, implemented in the model to get normal conditions. The Bituminous coal with given molar/mass fractions has for example a molecular weight of 10.45kg/kmol. Since the model operates with a coal feed of 1kmol the feed rate has the same value, 10.45kg/s. This numbers may be calculated, but in PRO/II it can be red directly from a chemical report. The amount of syngas is found by adding the molar fractions of CO and H_2 and multiply the numbers with the normalized amount of syngas. When the volume of syngas and the weight of the coal are known, the ratio Nm^3 syngas/ton coal can be set up. The values are comparable with the values found in literature.

The next step is to get the right amounts of oxygen and steam. The oxygen to syngas rate could be calculated directly from the chemical report at standard conditions since the correlation between Nm^3 and Sm^3 is the same for both gasses. The amount of oxygen is regulated to reach a close to real life rate, but not exceeding a realistic gasification temperature. A too high gasification temperature could be regulated with steam, but also here there are limits. Too much steam will cause too high water content in the product gas. The steam consumption is in literature calculated as kg steam/ Nm3 syngas. The chemical report gives the rate on mass basis and the amount of syngas at normal state is found using the same method as mentioned earlier. The same number could not be used since the change in input regarding to oxygen and steam also contributes to a change in the amount of syngas and in the composition.

These operations are repeated until acceptable levels of oxygen, steam, syngas composition and temperature are reached. The numbers are shown and discussed in chapter *4.2.3 PRO/II simulations*.

3.2.5   Chemical equilibrium calculator

In addition to PRO/II calculations there are done some direct calculations using an online chemical equilibrium calculator. The chemical equilibrium calculator gives the molar and mass fractions for given reactants at given temperatures and pressure. It is a tool where the users define two constant constraints among pressure, volume, temperature, entropy, enthalpy and internal energy. In this case constant volume and constant pressure are assumed. This is because in a gasifier the volume is fixed by the control volume. Constant pressure is also valid

since the reactants all are fed at the gasification pressure. There is be pressure loss in the gasification reaction, as in all other reactions, but this can be consider it as negligible for chemical equilibrium calculation purposes. The temperature is calculated using two initial values. The calculator names them *starting temperature* and *estimated equilibrium temperature*. The chemical equilibrium calculator handles coal in the same way as PRO/II, which means that the coal is defined as a mixture of C, H_2, O_2, S and N_2. The calculator also handles pure elements like H instead of H_2. It is therefore done calculations on both atomic and molecular level. On an atomic level the molar fraction differ since the molar weight is halved for the hydrogen, oxygen and nitrogen. Table 3.13 gives the fractions for this special case.

Table 3.13. Coal types on elementary basis.

Coal		Mol Fraction					
Region	Classification	C	H	O	N	S	H_2O
Rhein	Browncoal	0.471	0.387	0.137	0.003	0.002	0.000
Rhein with water		0,387	0.318	0.113	0.003	0.002	0.178
Datung	Bituminous	0.596	0.346	0.050	0.005	0.002	0.000
Ruhr	Anthracite	0.683	0.296	0.014	0.009	0.002	0.000

Molar fractions of the coal, H_2O and pure O_2 are given to the calculator and set to the same gasification pressure as in PRO/II. The gasification temperature is calculated in the program, and therefore some trial and failure among initial temperature and estimated equilibrium temperature is done to reach the same temperature as in the other model.

3.2.6 Water shift reforming

3.2.6.1 Water gas shift reactor

The procedure after the gasification is independent of the coal feed. The product gas contains much the same fractions of CO and H_2. In further calculation it is only focused on one coal. The principles are though the same for all the coals, with some minor modifications. The Bituminous coal from Datung, China, is studied through the rest of the calculations. This is a good coal for gasification and there are available literature about composition and heating values.

Between the gasifier and the water gas shift reactor (WGS) it is implemented a heat exchanger. The purpose of the heat exchangers is to lower the syngas temperature before the shift reactor. This is because a low temperature favors the H_2 production rate. The WGS is modeled in two steps. A high temperature shift and a low temperature shift. In PRO/II there is defined an equilibrium reactor which can be modified for different purposes. The default reactions for a reactor like this are the methanation reaction and the water shift reaction. The WGS is implemented because the goal in the model is to produce hydrogen.

In the shift reactors CO and H_2O forms H_2 and CO_2. An additional steam supply is needed to convert as much as possible of the CO. The principles of the water reactors are shown in figure 3.14.
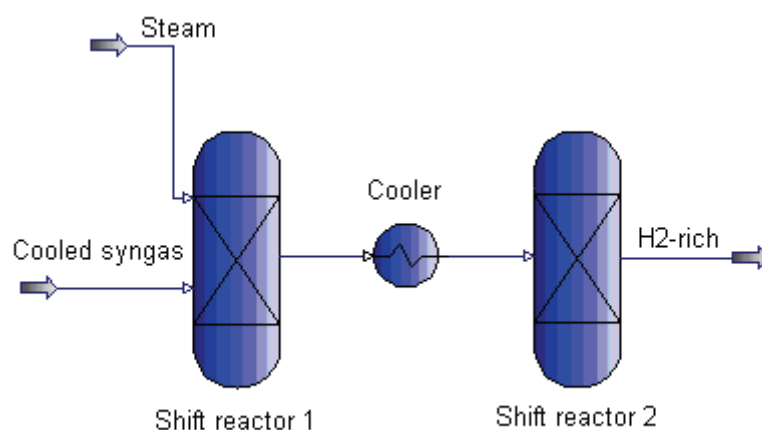
Figure 3.14. Two stepped water gas shift reactor.

There is put no duty on the equilibrium reactors. The cooled syngas is fed at 250°C and 41.4bar. The stream comes from the gasifier and was cooled with a heat exchanger because this favors the H_2 production and the conversion of CO to CO_2. Water steam is fed to the first stage at about 255°C. The amount of steam is discussed in *4.2.5.1 Water gas shift reactor*. According to literature the H_2O/CO rate is supposed to be 1.4-2.0 [21]. It differs depending on the amount of coal fed to the gasifier, which again is decided from the wanted fuel amount in the power cycle. After the first stage the product stream is cooled to 225°C before it enters the second stage. The product stream from the second stage has to be in vapor phase to be sure that the reactions have occurred [27]. That is the reason why the water feed temperature not is even lower. If the water condenses the reactions may occur, but not for sure. In both the gasifier and in the shift reactors the pressure drop is set to 0.4bar.

It is normal to demand a CO conversion rate that returns a H_2 rich gas out of the shift reactor with a CO content of about 2 percent. With no duty on the reactor the vapor feed is used as cooling water to achieve low enough temperature to reach the goal of 2 percent CO. Without duty on the equilibrium reactor it is impossible to reach this value in one step without very high steam consumption. Steam is expensive to produce and has a high utility value. A very high steam concentration in the H_2 rich gas will as mentioned affect the turbine negatively. It is therefore installed another low temperature stage. This is considered as a better solution than putting duty on the reactor. A heat exchanger between the stages gives potential for heat integration with the steam cycle in the Power Island. Compressed cooling water may be superheated in the heat exchanger and support the steam cycle. With this integration the exothermic reactions in the WGS can be utilized to generate steam instead of consuming steam. With a heat exchanger between the two stages and water supply at the second stage the production is satisfactory regarding to CO concentration. A low concentration of CO indicates that the carbon is shifted to CO_2 and can be captured. Both the heat from the first and the second stage may be cooled and utilized to produce steam. This is discussed more in *4.4.2.2 Adding steam to the steam turbine*.

3.2.6.2   Integrating gasification and water gas shift

There is made a model that integrates the gasifier with the shift reactors in a way where the water feed could be regulated between the stages. With a constant water supply for the whole island, a splitter is installed to regulate the water feed between the gasifier and the shift reactor. For example, more steam could be fed to the gasifier to lower the temperature. This will result in a higher water fraction in the syngas. Then the additional water supply in the shift reactor could be reduced. This model is shown in figure 3.15**.**
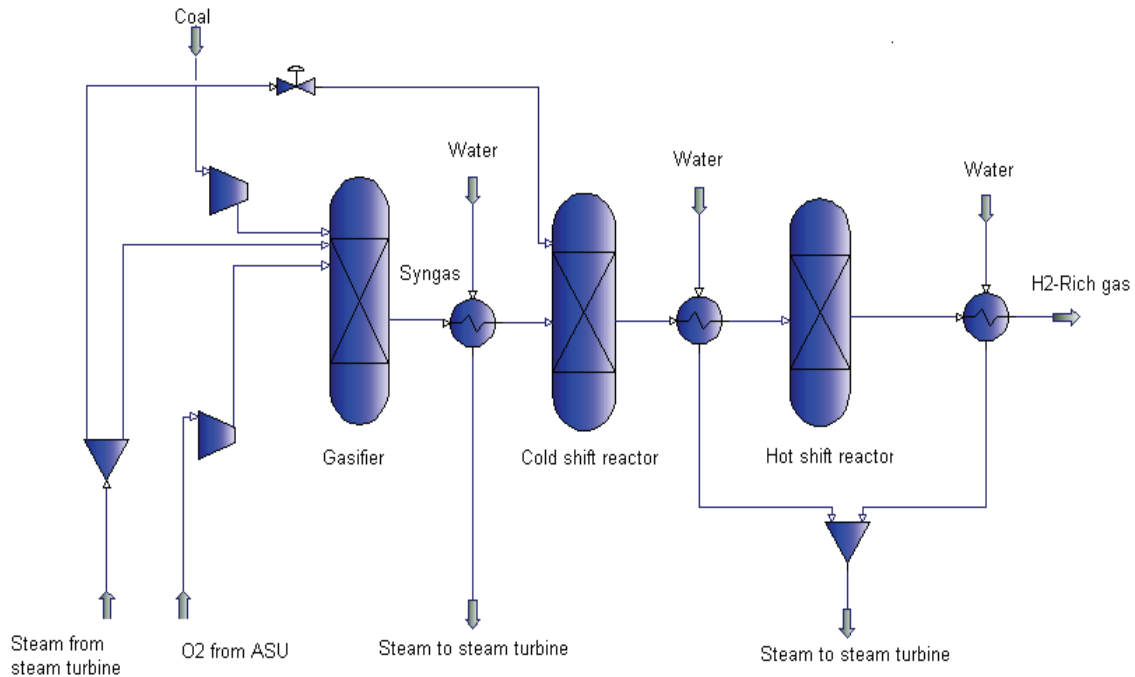
Figure 3.15. Model of Gasification Island.

The heat exchangers cool the gas at the different stages and then get the water gas shift reaction in favor of H_2 and CO_2. The heat is utilized to generate steam to the Power Island. This compensates for some of the exothermal heat losses in the gasification process and in the shift reaction. This means that the heat is recovered in the HRSG in the Power Island.

Calculations on heating values are done using LHV. The coals had tabulated heating values. In this case the LHV is calculated manually using Kay's rule. This is because the coal in the model acts like a mixture and not a complete coal. The heating values are calculated from equation 3.23, using C, H_2 and S as the only heating value carrying substances.

$$LHV_{coal} = n_C \cdot LHV_C + n_{H_2} \cdot LHV_H + n_S \cdot LHV_S \qquad (3.23)$$

The same principle is used finding the heating value for the syngas and the H_2 rich gas, but here the CO and H_2 are the only substances with heating values.

3.3 Acid Gas Removal

3.3.1 Simulation tool

There are not performed any simulations on an acid gas remover. To calculate the energy demand of the island, capture costs based on energy consumption per captured amount of carbon dioxide is used. The calculations are done in Microsoft Excel.

Stream properties out of the AGR unit are also calculated in Microsoft Excel. The fuel composition into the unit is calculated in *3.2 Gasification Island* and with a capture efficiency presented in the subsequent section the cleaned fuel stream is found.

3.3.2 CO_2 capture unit

When choosing a CO_2 capture process, the partial pressure of carbon dioxide and the scale of the plant are important decision factors. An IGCC plant is in most occasions considered as large scale plants and the capture process chosen need to handle large amounts of CO_2. The fuel gas from the water gas shift reactor contains mainly hydrogen and carbon dioxide. The distribution is on dry basis 58.2% H_2, 39.0% CO_2, 2.4% CO, 0.2% N_2 and 0.1% H_2S. The pressure after the shift reactor is at 40.2bar. This gives a partial pressure of carbon dioxide of about 15.7bar which is considered as high.

On behalf of the large scale of the plant and the high CO_2 partial pressure it is decided to use an absorber in the capture process. Because of the relatively high pressure in the fuel stream physical absorption is preferred before chemical absorption [21].

In this report there are not done any simulations or tests on the CO_2 capture unit. A capture method is chosen and energy consumption per kilogram captured carbon dioxide is used to calculate plant efficiency reduction and unit energy consumption.

The gasifier chosen in *3.2 Gasification Island* is an entrained flow gasifier. The most common entrained flow gasifier is the shell gasifier. The gas from a shell gasifier performs desirable with selexol used as solvent in a physical absorption process. The following key numbers are therefore used in further calculations on the acid gas remover.

Table 3.14. Properties of the Acid Gas Remover [21].

Gasification method	Shell
CO_2 capture technology	Physical absorption
CO_2/H_2 separation method	Selexol
CO_2 capture ratio	96 %
CO_2 scrubbing cost	0.06-0.11 kWh/kg CO_2 captured
CO_2 compression cost	0.11-0.13 kWh/kg CO_2 captured

The total amount of captured carbon dioxide must be found to calculate the total energy consumption in the acid gas remover. This is done in the calculations of the entire IGCC plant.

The scrubbing cost presented in table 3.14 is mainly the cost of pressurize the solvent to fuel gas pressure. The solvent is sent to the fuel gas and the CO_2 is absorbed to the selexol. Selexol with attached carbon dioxide is then removed from the fuel gas. The separation of selexol and CO_2 is done by expansion to atmospheric pressure. Then the selexol is regenerated and the carbon dioxide must be compressed to a desirable storage pressure. The compression cost of a pressure rise to 110bar is given in table 3.14. This energy demand must be implemented in the total energy cost calculation of CO_2 capture.

The capture ratio of CO_2 is also given in table 3.14. 96% of the carbon dioxide is led out of the black box in a separate stream. The remaining CO_2 is sent to the turbine together with H_2 and the other substances in the fuel gas. As an end product with no heating value, the carbon dioxide is inert and do not react in the combustion chamber. The remaining 4% of the CO_2 is therefore emitted to the environment.

Figure 3.16 in *3.3.2 H₂S capture unit* is showing a black box overview and table 3.15 is giving the stream properties.

3.3.3   *H₂S capture unit*

The fuel gas from the water gas shift reactor consists also of small amounts of hydrogen sulfide. The hydrogen sulfide is removed in the same scrubbing process as the carbon dioxide. The physical absorption process removes CO_2, H_2S, COS, organic S-compounds, HCN, aromatic compounds and higher hydrocarbons [21]. There is therefore no cost of hydrogen sulfide removal from the fuel gas in addition to the cost mentioned for CO_2 removal. After the scrubber, the hydrogen sulfide is brought back to elementary sulfur in the Claus process. This is not further discussed in the report.

Table 3.16 shows the stream properties and figure 3.16 gives a unit overview of the scrubber handling both CO_2 and H_2S capture.
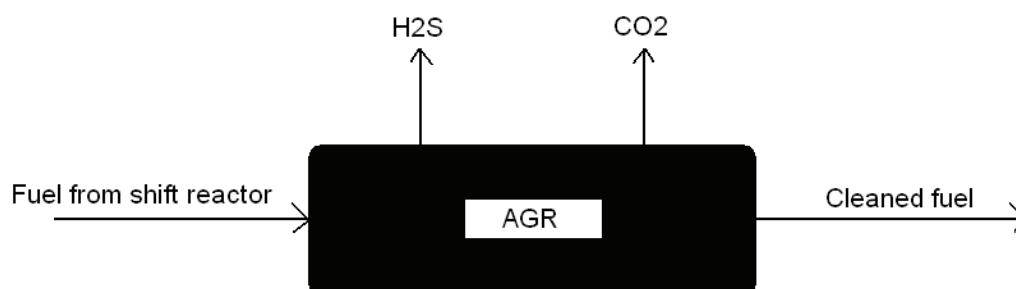
Figure 3.16. AGR black box.

Table 3.15. AGR stream properties.

Stream description	Fuel from WGS	Dry fuel	Cleaned fuel	CO₂-stream
Flowrate	2.167	1.772	1.106	0.666
Composition				
C	0.000	0.000	0.000	0.000
CO	0.020	0.024	0.039	0.000
CO₂	0.319	0.390	0.025	0.997
O₂	0.000	0.000	0.000	0.000
H₂	0.476	0.582	0.933	0.000
H₂O	0.182	0.000	0.000	0.000
CH₄	0.000	0.000	0.000	0.000
N₂	0.002	0.002	0.003	0.000
NO	0.000	0.000	0.000	0.000
S	0.000	0.000	0.000	0.000
SO₂	0.000	0.000	0.000	0.000
H₂S	0.001	0.001	0.000	0.003

It is assumed no leakage of H_2 or other substances in the CO_2 and H_2S stream. In a real plant there will probably be some minor amounts of the other substances in the waste streams reducing the fuel stream.

3.4   Power Island

3.4.1   Simulation tool

To model the Power Island GT PRO 18.0 is used. This is a computer tool developed for modeling of gas fired power plants. It also includes the steam cycle in a combined cycle. First the gas cycle is presented.

The modeling procedure presented in this report is very simplified. A lot of the values in the calculations are based on default numbers in the program. The goal with this model is to calculate power output and the fuel consumption. It is important to know the required fuel consumption for the gasification model. This will again give the needed amount of oxygen and steam from the air separation unit and HRSG.

The model is based on an ambient temperature of 298K, a pressure of 1.0009bar at altitude 109.6 meters above sea level and a relative humidity of 60 %. The altitude and the pressure correspond to the numbers of Heidelberg, Germany. This location is chosen due to the possibility of building an IGCC in central Europe is higher than northern Europe. Choosing northern Europe instead will although not lead to large derogation compared to central Europe. The temperature of 298K equals a hot summer day which is a conservative assumption compared to winter ambient conditions. 298K is used in the ASU and the gasification as well.

3.4.2   Gas Turbine

The gas turbine type chosen is the Siemens SGT5-4000F. This model is presented in *2.4.3 Turbines fired with hydrogen,* and according to Siemens the new models of this type are fitted to handle hydrogen rich fuel. Most of the theory treats with the SGT6-5000F model, but it is assumed that the chosen turbine can operate under similar conditions. SGT5-4000F is chosen to get the wanted 50Hz on the European power grid. The chosen turbine has characteristics presented in table 3.16.

Table 3.16. SGT5-4000F properties.

Shafts	1
Rounds per minute	3000
Pressure rate	16,2
Turbine inlet temperature [K]	1583
Exhaust temperature [K]	844
Air Flow [kg/s]	617
Power [kW]	232400

The H_2 rich gas from the Gasification Island is chosen as fuel. It is not ran any simulations on a syngas turbine since the Gasification Island includes a shift reactor and a CO_2/H_2S scrubber.

3.4.2.1 Feeding hydrogen rich fuel to the turbine

The fuel composition is based on the product stream from the Gasification Island. Before the CO_2/H_2S removal the water is condensed. As mentioned in chapter *3.3.2 CO$_2$ capture unit*, 96% of the CO_2 and all the H_2S are removed. Excel is used to calculate the composition of the feed when water is condensed and the CO_2/H_2S scrubber is implemented. The compositions are shown in table 3.17.

Table 3.17. Compositions of the fuel on different stages.

Stream Name		H2-rich gas	Dry gas	After CO_2/H_2S removal
Phase		Vapor	Vapor	Vapor
Temperature	C	294.134	36.670	25.000
Pressure	Bar	40.400	40.200	40.000
Flowrate	kmol/s	1.097	1.070	2.167
C		0.000	0.000	0.000
CO		0.020	0.024	0.039
CO_2		0.319	0.390	0.025
O_2		0.000	0.000	0.000
H_2		0.476	0.582	0.933
H_2O		0.182	0.000	0.000
CH_4		0.000	0.000	0.000
N_2		0.002	0.002	0.003
NO		0.000	0.000	0.000
S		0.000	0.000	0.000
SO_2		0.000	0.000	0.000
H_2S		0.001	0.001	0.000

The temperature levels here are results from PRO/II simulations including heat exchangers used to utilize the heat removed. This is discussed closer in *4.4.2.2 Adding steam to the steam*

turbine. There is still some CO_2 in the mass flow. The carbon dioxide act as an inert and increase the mass flow through the turbine. So for the power production it is not negative, but it will lead to a small CO_2 emission. The CO contains heating value and is converted to CO_2 in the combustion process. Because of the very high fraction of H_2 the fuel stream is diluted with nitrogen from the Air Separation Island.

In ordinary gas turbines water steam can be utilized as a diluter. For hydrogen turbines this is not the case. It contributes to higher moisture in the turbine that again affects the heat transfer and put more strain on the materials. When also CO_2 capture is included the water removal contributes to a higher fraction of CO_2 before the removing process.

Table 2.7 in *2.4.3 Turbines fired with hydrogen* shows that the chosen turbine can handle a hydrogen fraction at 70 % and even higher. It is therefore run a simulation with 70 % H_2 with N_2 used as an extra diluter in addition to the small CO_2 amounts. That gave a relatively low demand of nitrogen. Nitrogen is available from the ASU. The ASU produces the required amount of oxygen for the gasification process and this gives a considerable amount of N_2. It is therefore beneficial to consume this nitrogen in the turbine to increase the mass flow and regulate the temperature. GTPRO gives the required mass fraction for each fuel composition. The wanted amount of hydrogen can then be calculated. When the required amount of hydrogen is calculated, the necessary amount of oxygen for the given coal in the given gasifier is found. That amount of O_2 will again give the amount of N_2 that is produced for the given amount of O_2 in the ASU.

The 70% H_2 fuel gave a considerable lower N_2 demand than the appurtenant production of N_2 in the ASU based on the O_2 demand for the gasification. The N_2 amount is therefore increased. When increasing the N_2 amount in the fuel flow it is important to keep the same scale between the other substances so the overall mass balance is correct. This is done in Excel. Several iterations are performed to get a suitable amount of hydrogen and nitrogen that corresponded to the O_2/N_2 production in the ASU. The final composition of fuel diluted with N_2 is shown in table 3.18.

Table 3.18. Fuel composition.

Stream Name	Diluted with N_2
Phase	Vapor
Temperature	25.000
Pressure	26.260
Flowrate	2.167
CO	0.021
CO_2	0.014
H_2	0.504
H_2O	0.000
N_2	0.461

Table 3.18 only shows the fractions that are fed as fuel into the turbine. The absolute values and other results are described in *4.4.1.2 Nitrogen, hydrogen and oxygen demand*. GTPRO gives no warning using this fuel composition in a normal combined cycle. GTPRO also has a gasification function, but this function is only used to check what happened when feeding syngas to the turbine. GTPRO then suggested increasing the turbine nozzle area with 6%. It can be assumed that the same is necessary for a hydrogen rich fuel.

This composition is now fed to the combustion chamber. The most important calculation is to find the fuel consumption since this gives the wanted H_2 productions in the Gasification Island, and the required amount of O_2. Emphasize is put on this since the ASU and the Gasification Island are the major parts of this report.

3.4.3   *HRSG and Steam Turbine*

The power cycle is simulated in GTPRO while the Gasification Island is modeled in PRO//II. Integrating the two processes is done by manual iterations between the two simulation tools. The goal is to use the surplus heat from the Gasification Island to generate more steam. This steam can be utilized in the steam cycle to increase the power output. In addition, steam from the steam turbine is taken out to cover the need of steam in the Gasification Island internal.

It is chosen one evaporation pressure in the Heat Recovery Steam Generator (HRSG). The inlet pressure and inlet temperature for the steam turbine is chosen using the default values in GTPRO. That gives 83bar and 792K.

3.4.3.1   Utilizing steam from the steam turbine

Steam is also utilized in the gasifier and the water shift reactors as a reactant in the processes. The steam needed for the gasification is extracted from the steam turbine at the wanted pressure and temperature, in this case 42bar and 255˚C. The amount etc is discussed closer in *4.4.2.1 Utilizing steam from the steam turbine.*

3.4.3.2   Adding steam to the steam turbine

To find the amount of steam that can be generated from the Gasification Island it is made sub models in PRO/II. These models use the different heat sources to generated steam. Four sources are utilized in steam generating, the exhaust gas from the Power Island, the syngas, the gas between the shift reactor stages and the H_2-rich gas. The last one is cooled to condense and remove the water. The exhaust gas from the Power Island has a temperature of 190˚C after the HRSG. This is utilized to preheat the water before it is superheated using the high temperature syngas. The procedure is shown in figure 3.17. The steam produced here is fed as high pressure steam to the steam turbine in GTPRO. The temperature and pressure is decided directly from GTPRO. The variable then becomes the mass flow. This is regulated until the syngas reached a temperature level of 250˚C, which is the wanted inlet temperature for the water gas shift reactor.
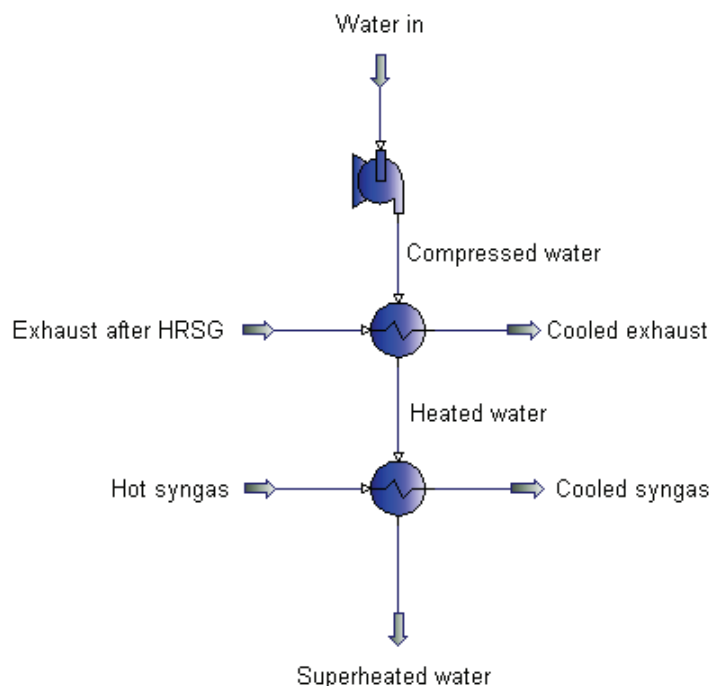
Figure 3.17. Generating steam from exhaust gas and hot syngas.

The process illustrated in figure 3.17 is used to produce high pressure steam. Two other heat integrations are also performed, then to produce low pressure steam. The first one is for cooling the gas between the two stages in the shift reactor. This is shown in figure 3.18.
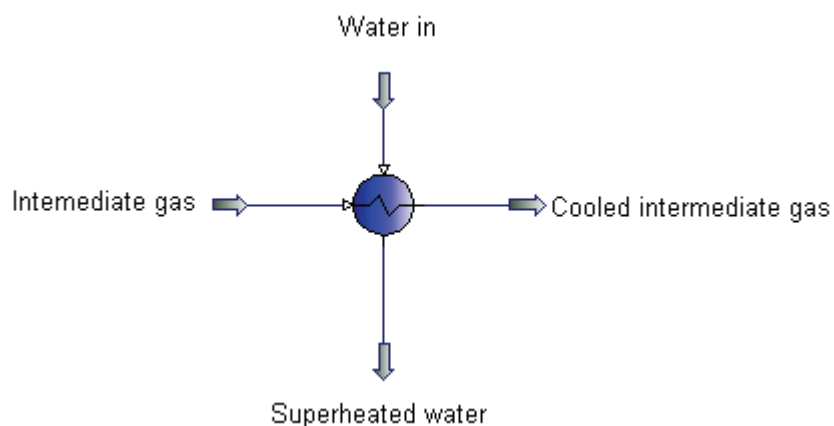
Figure 3.18. Generating steam between the stages in the shift reactor.

The last integration is used to condense the water vapor in the H_2-rich gas after the last step of the Gasification Island. This is illustrated in figure 3.19.
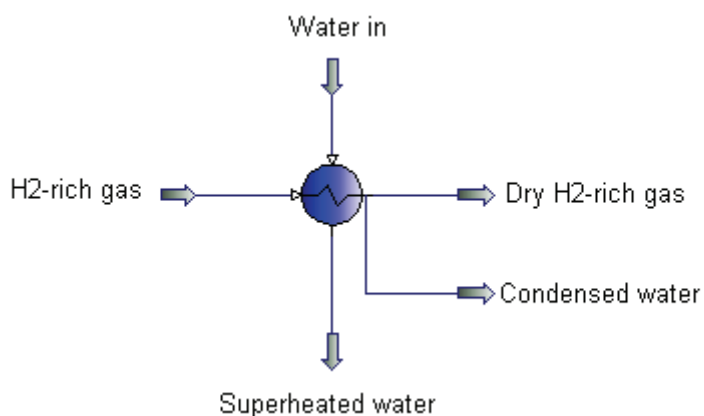
Figure 3.19. Generating steam after the shift reactor.

The procedure of integrating steam from the Gasification Island is presented in this chapter. The amount of steam, the temperature/pressure and the power output is presented and discussed in *4.4.2.2 Adding steam to the steam turbine*.

3.5 IGCC Power Plant

3.5.1 Integrating the whole plant

The whole plant including Air Separation Island, Gasification Island, Acid Gas Removal and Power Island is put together manually using Excel and calculations by hand. This is a bit challenging since the ASU and the Gasification Island are simulated in PRO/II and the Power Island is modeled in GTPRO. The Acid Gas Removal is done manually. This chapter gives a quick introduction to the integration process between the islands and simulation tools. The main points are already described in *3.4 Power Island* and the results are discussed in *4.5 IGCC Power Plant*.

3.5.1.1 Integrating the gas cycle

When integrating the gas cycle the challenge is to fit the required amounts of fuel with the Gasification Island and then the ASU. The fuel is fed as a mixture shown in table 3.19**.** To find this fuel composition iterations are done to fit the N_2 production decided by the O_2 production required to produce the wanted amount of H_2 in the Gasification Island.

3.5.1.2. Integrating the steam cycle

The steam cycle is integrated with the Gasification Island to recover the heat released from the reactors and utilize it to produce more steam. In addition the steam needed in the gasification process is taken from the steam turbine at 42bar and 255°C to cover steam needs internally. These integrations are explained in *3.4.2 HRSG and Steam turbine*.

4 Results and Discussion

4.1 Air Separation Island

4.1.1 Gaseous oxygen

In this part of the report, results achieved in the PRO/II models presented in *3.1. Air Separation Island* are discussed. The results of the GOX plant are first analyzed and optimized. Variations and sensitivity are discussed. Afterwards the produced oxygen is compressed to compare the GOX and LOX plant.

4.1.1.1 Energy consumption considerations

A figure of the initial developed GOX plant is shown in figure 3.8 in *3.1.2.8 After treatment of oxygen and nitrogen*. Stream properties for all the streams in the model are given in Appendix E.

The only work added to the island is the compressor work of the four compressors forming the main air compressor. The properties of the compressors are given in table 3.2 first shown in *3.1.2.2 Air cleaning*.

Table 3.2. Compressor work of compressing 0.99 kmol of dry air.

Compressor Name			C1	C2	C3	C4
Pressure	bar		1.60	2.50	4.00	6.43
Temperature	K		348.94	348.39	351.33	351.91
Head	m		5224	5167	5468	5526
Actual Work	kW		1469	1453	1538	1554
Isentropic coef.. k			1.4013	1.4024	1.4041	1.407

By adding the compressor work from the compressors it is found that the total work is 6014kW. The optimal distribution of work is from theory achieved when the compressors

have equal work. It is although found that the work is slightly lower when the two first compressors have a little lower individual work than the two last ones [10].

The distribution of work done by compressors given in table 3.2 is found by trying and failure method. The total work done by the compressors might be a little more optimized by further trying and failure with other pressure levels. The solution given is although near optimal and close enough for the purpose of this report.

As mentioned in *3.1.2.2 Air cleaning,* the amount of air compressed is 0.99kmol. This is because of the assumption of one mole percent of water vapor content in air. To use a splitter to model the molecular sieves and include the water vapor content in air through the compressors intuitive seems like the optimal solution. This is unfortunately not possible due to limitations in PRO/II. Therefore the compression of the water vapor needs to be calculated separately and added on the dry air compression work. The additional work is estimated by a simple calculation.

$$\frac{0.01 kmol_{H_2O}}{0.99 kmol_{Air}} \cdot 6014 kW \cdot \frac{18.02 kg/kmol_{H_2O}}{28.96 kg/kmol_{Air}} = 38 kW \tag{4.1}$$

This is a simplification of the actual process. To get an exact value for the additional work, condensation of water vapor should be included. The content of water vapor in the air is not influentially large, and a simplified estimate of additional work is good enough.

The total work done by the main air compressor is then 6052kW for 1kmol of moist air.

To draw conclusions of the GOX plant, the incoming air stream and the outgoing oxygen and nitrogen streams need to be analyzed. The streams are shown in table 4.1.

Table 4.1. Incoming and outgoing streams of the GOX plant.

Stream Name		A1	OX9	NI8
Phase		Vapor	Vapor	Vapor
Temperature	K	298.000	296.977	297.000
Pressure	bar	1.000	1.500	1.000
Flowrate	kmol/s	0.990	0.216	0.774
Composition				
O_2		0.210	0.956	0.002
N_2		0.781	0.011	0.996
AR		0.009	0.033	0.002

Stream A1 is the air inlet of the island. OX9 and NI8 is respectively the oxygen and the nitrogen produced.

The specifications set in the columns are minimum 95% purity in the oxygen stream and minimum 99% purity in the nitrogen stream. With 95.6% oxygen in OX9 and 99.6% nitrogen in NI8 this is maintained.

The most important factor in an ASU after achieved the wanted purity is the energy consumption. To compare different production rates and technologies this is normally given in energy consumption per produced kilogram of oxygen. For the GOX plant the calculated energy consumption is given by 4.2.

$$\frac{6052kW}{0.216kmol/s \bullet 0.956kmol_{O_2}/kmol \bullet 32.00kg_{O_2}/kmol_{O_2} \bullet 3600s/h} = 0.254kW/kg_{O_2} \quad (4.2)$$

To be able to compare numbers for air separation plants with different oxygen purity, the unit of the energy consumption is in pure oxygen.

The GOX plant delivers oxygen requiring 0.254kW per kilogram of oxygen. Conventional air separation plants produce oxygen at an energy price of 0.25kW per kilogram oxygen and modern facilities have a production costs down to 0.22. The model developed is thereby on a satisfying energy consumption level, but improvements are possible.

4.1.1.2   Pressure considerations

To optimize the model, the compression work of the main air compressor must be decreased. There are two ways to this, either by lower the inlet pressure of the high pressure column or to install better equipments with lower pressure losses before the entrance of the first distillation column. Decreasing of the pressure in the high pressure column has direct impact of the temperatures of the streams out of the column. A pressure reduction leads to a lower temperature of stream NI1 which gives the temperature for the heat stream in the combined condenser and reboiler. This temperature has to be above the cold stream OX3 entering the combined condenser and reboiler. NI1 has to be not only above OX3, but enough above to satisfy the given constraint of ΔT at 1K.

Table 4.2 gives stream NI1 and OX3 for the initial pressure in the top of the column of 5.5 bar and the streams with a pressure reduction of 0.5bar to 5.0bar.

Table 4.2. Stream properties for pressure change in the high pressure column.

Stream Name		NI1	OX3	NI1	OX3
Phase		Vapor	Liquid	Vapor	Liquid
Temperature	K	95.338	93.642	94.126	93.485
Pressure	bar	5.500	1.500	5.000	1.500
Flowrate	kmol/s	0.437	0.447	0.365	0.344
Composition					
O_2		0.005	0.950	0.006	0.950
N_2		0.990	0.014	0.990	0.020
AR		0.005	0.036	0.004	0.030

Table 4.2 shows that the ΔT is reduced from 1.696K to 0.641K for the 0.5bar pressure drop. Having only 0.641K in temperature difference in the combined condenser and reboiler is indeed possible, but it requires better and more expensive heat exchanging equipment. If this investment is done the compression work is reduced to about 5800 kW. There are also some minor changes in the outgoing oxygen composition and the new energy consumption per kilogram produced oxygen is given by 4.3.

$$\frac{5786kW}{0.213kmol\,/\,s\bullet0.957kmol_{O_2}\,/\,kmol\bullet32.00kg_{O_2}\,/\,kmol_{O_2}\bullet3600s\,/\,h} = 0.246kW\,/\,kg_{O_2}\quad(4.3)$$

Stream properties and compressor work for this case is given in Appendix F.

Equation 4.3 shows a reduction in energy consumption per kilogram oxygen produced that have to be taken into account when the quality of the heat transfer equipment in the combined condenser and reboiler is economical analyzed.

The optimal solution is to find a minimized top column pressure level which also maintains the ΔT demand of 1K. This is discussed further in *4.1.1.6 Overall GOX considerations*.

It is of course also possible to lower the bottom pressure in the low pressure column, here given by OX3, instead of the top pressure of the high pressure column. The problem with this is that the pressure in OX3 is difficult to get lower. A lower pressure in OX3 would demand an even lower pressure in the top of the low pressure column where the pressure already is near ambient.

Another option to lower the compressor work is to decrease the pressure losses before the high pressure column. The aftercoolers in the main compressor have a pressure loss of 2-3 percent. The pressure loss between the last air compressor and the high pressure column is initially 0.3bar. This is about 5% and covers both the pressure drop in the main heat exchanger and in the molecular sieves. These losses are difficult to optimize further, but small improvements can be made. The improvements are not as large as the ones for column pressure reductions. This is because the pressure losses are smaller than the pressure reduction in the high pressure column.

It is also possible to decrease the total work by reduction of the pressure losses in the columns. The pressure loss is set to 0.5bar in both the HP and LP column. In the HP column this equals a loss of 8.3 percent and a reduction here is directly leading to a lower compression work. In the LP column the same 0.5bar pressure loss gives a considerable loss in the column. The LP column pressure loss is higher because of several incoming and outgoing streams compared with the HP column. Lower pressure loss here gives only indirect reduction of compressor work. A reduction of LP column losses gives either lower reboiler pressure or higher top tray pressure or a combination of these. Lower reboiler pressure leads to lower temperature which gives higher temperature difference between OX3 and NI1.

Higher top tray pressure does not give any direct energy advantages, but is necessary to "push" the nitrogen stream out of the ASU.

The pressure adjustments are also influencing the purity levels. All changes have impact on each other and the final pressure solution is presented in *4.1.1.6 Overall GOX considerations*.

4.1.1.3   Change in the main heat exchanger

As mentioned in *3.1.2.3 Main heat exchanger* in the method the model of the main heat exchanger is a little different than the theory presented in *2.1.2.4 Main heat exchanger* in the theoretical background. In the theory the stream to the low pressure column is taken out somewhere inside the main heat exchanger and the pressure is decreased by an expander. In the model presented the main air stream is split in two streams after the main heat exchanger, A9-2 at 0.09kmol/s choked and fed to the low pressure column and A9-1 at 0.90kmol/s fed directly to the high pressure column. Because A9-2 is cooled through the whole main heat exchanger there is no need for an expander before the low pressure column, and the temperature of A10-2 is decreased enough by a valve.

From table 4.1 the properties of the outgoing oxygen and nitrogen stream are presented. With a ΔT at 1K and ambient assumptions of 298K, OX9 and NI8 are at their maximal temperature at 297K. In air separation for IGCC application, it is favorable to have a high temperature of the oxygen stream and a low temperature of the nitrogen stream. The oxygen is used in the gasifier and hot oxygen uses less energy from the coal to achieve gasification temperature. The nitrogen is utilized as a fuel diluter in the power cycle. Low temperature of the nitrogen gives lower fuel temperature and higher temperature differences in the turbine. This again leads to more power output.

It is not possible to raise the oxygen temperature in the ASU without removing aftercoolers. This is not efficient and the maximal temperature of OX9 is the already achieved 297K. By changing the main heat exchanger NI8 may not be heated as much as the original model and the nitrogen to the power island can be at a lower temperature.

This is done by leading the small air flow to the low pressure column out of the main heat exchanger before it is entirely cooled, and use an expander instead of a valve to remove more energy from the stream. This is shown in figure 4.1.
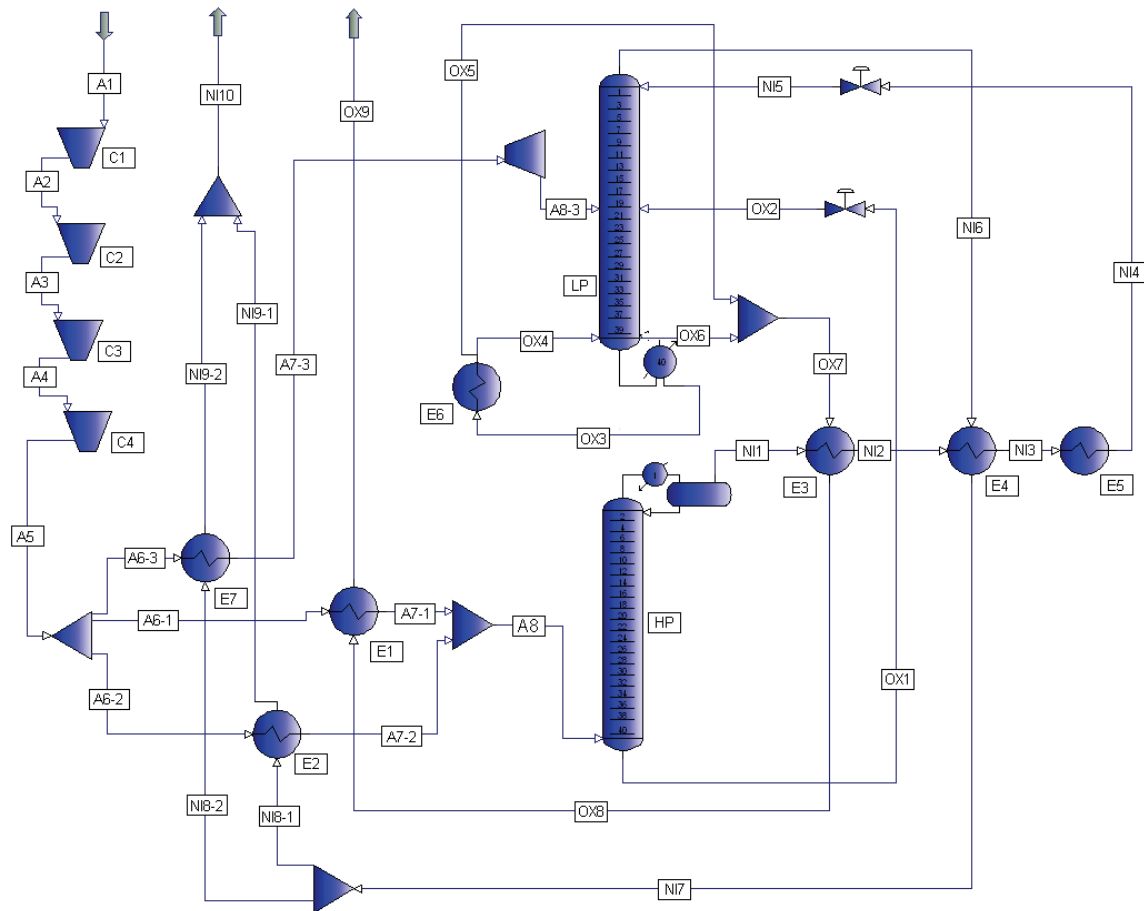
Figure 4.1. Model of GOX plant with changed main heat exchanger.

This model has approximately equal stream properties as the previous GOX model. The compressor work is equal and the purity of the products is close to equal.

The splitter in the main heat exchanger is adjusted to cool the nitrogen stream as much as possible and at the same time maintain the work added and purity of the outgoing streams. Stream properties for all the streams in the model are given in Appendix G and the outgoing streams OX9 and NI10 is presented in table 4.3

Table 4.3. Stream properties for modifications in main heat exchanger.

Stream Name		A1	OX9	NI10
Phase		Vapor	Vapor	Vapor
Temperature	K	298.000	297.000	288.803
Pressure	bar	1.000	1.500	1.000
Flowrate	kmol/s	0.990	0.215	0.774
Composition				
O_2		0.210	0.956	0.002
N_2		0.781	0.011	0.996
AR		0.009	0.033	0.002

Compared to table 4.2, table 4.3 shows a decrease of temperature in the outgoing nitrogen stream of 8.2K. This temperature reduction has no energy cost and no energy demand. The only change is the air stream split to the low pressure column. This is handled inside instead of after the main heat exchanger, and there is used an expander instead of a valve for pressure reduction.

To find the energy advantage of having nitrogen at 289K instead of 297K a power cycle analysis must be done. To decide if this is economic feasible, the energy surplus and the investment costs of the more complex main heat exchanger and expander instead of valve must be analyzed. This is not done here.

It is not easy to lower the compression work by changing the main heat exchanger. This is because of the pressure dependent temperatures in the combined condenser and reboiler is the deciding factor of the compressor work. The main advantage of this change is as mentioned the reduced nitrogen temperature.

4.1.1.4   Investment costs considerations

As mentioned in *3.1.2.1 Compression* it was decided to model the main air compressor with 4 individual compressors. To decide this, a sensitivity analysis of the change in total work for different numbers of compressors is made. A simple example viewing the total work of compressing 1kmol/s of air from 1bar to 6.43bar for respectively 1 to 6 compressor steps is shown in figure 4.2.
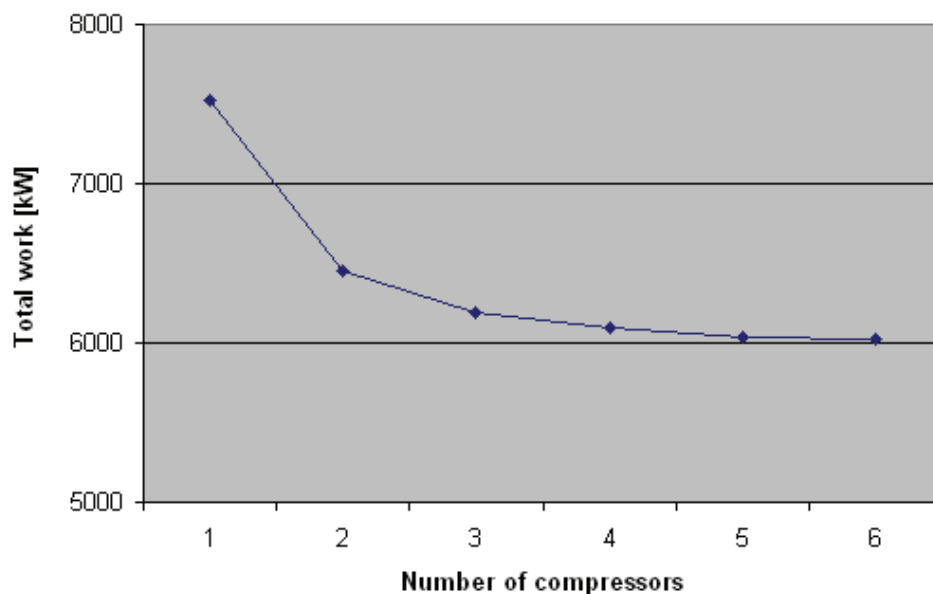
Figure 4.2. Decrease of total work with increasing compressor steps.

In Appendix H the calculations made to draw figure 4.2 is given.

Figure 4.2 shows a decrease in total work for an increasing number of compressors. It is decided to use 4 compressors to handle the pressure raise. Using a fifth compressor will lead to some reduced energy costs, but probably not enough to justify the investment expenses. Investing in only three compressors will on the other hand probably lead to an unacceptable high energy demand.

Table 4.4 gives the total work for compression of 1kmol/s of dry air for different number of compressors and the changes this will have for the energy consumption per kilogram produced oxygen. The air separation island used for the calculation is the initial GOX plant. This calculation assumes 1kmol/s of dry air instead of moist air, but the minor derogation from this is about the same for different compressor numbers. Calculations are given in Appendix H.

Table 4.4. Energy consumption for different number of compressors.

Number of compressors	[kW]	[kW/kg$_{O2}$]
1	7522	0.3126
2	6451	0.2712
3	6193	0.2603
4	6096	0.2563
5	6038	0.2538
6	6024	0.2532

The production cost of oxygen is not remarkable reduced from 4 to 5 compressors. Changing from 3 to 4 compressors gives a slightly larger reduction and the decision of 4 compressors is kept.

Another issue with concern to investment costs is the number of trays in the columns. Having many trays in a column makes the column physical larger and thereby more expensive. Both the columns have specifications concerning purity of the outgoing streams. The high pressure column has nitrogen purity specification and the low pressure column has oxygen purity specification. The number of trays for a given purity specification has influence on the condenser and reboiler duty. With fewer trays in the high pressure column the condenser duty increases. This leads to an increase in reboiler duty in the low pressure column since the condenser and reboiler is connected. Because of the reboiler duty is increased, there may also be fewer trays in the low pressure column.

Even though a reduction in number of trays in the high pressure column leads to a reduction in number of trays in the low pressure column it is not possible to have only 2 or 3 trays in each column. If the number of trays is decreased to much, the combined condenser and reboiler is not able to maintain the specified purity levels. The optimal solution is to find the minimal number of trays in the two columns that give equal condenser and reboiler duty, and at the same time maintain the specified purity levels.

This is done by removing trays from the columns stepwise. The removal steps in the high pressure and low pressure column must be adjusted to each other since the condenser and reboiler is connected and has equal duty. Between each step the purity levels must be checked and maintained.

The optimal solution is found when the high pressure column has 11 trays and the low pressure column has 16 trays. At this point the nitrogen purity is at the exact specified level of 99.0%. If the high pressure column has a further reduction of trays, the nitrogen purity is decreased below 99 percent and the specified purity is not maintained. The number of trays in the low pressure column is adjusted to the duty in the combined condenser and reboiler and still delivers oxygen at a purity level of 95.6%. A further reduction in number of trays in the low pressure column would not lead to purity problems, but leads to an energy demand in the reboiler larger than the energy delivered from the condenser. This had to be covered external and a further reduction below 16 trays is therefore not made.

Table 4.5 gives the incoming air stream and the outgoing streams OX9 and NI8 for the minimized number of trays.

Table 4.5. Stream properties with minimized number of trays.

Stream Name		A1	OX9	NI8
Phase		Vapor	Vapor	Vapor
Temperature	K	298.000	297.000	297.000
Pressure	bar	1.000	1.500	1.000
Flowrate	kmol/s	0.990	0.211	0.778
Composition				
O_2		0.210	0.956	0.007
N_2		0.781	0.011	0.990
AR		0.009	0.033	0.003

Stream properties for all the streams in the model with minimized number of trays are given in Appendix I.

This modification does not lead to any external energy demand. The oxygen purity is also maintained compared to the model with 40 trays on each column. The change is the small decrease of nitrogen purity in NI8. The energy consumption per kilogram oxygen produced is a little reduced due to more oxygen in NI9 and thereby a lower flowrate in OX9. The energy consumption per kg of produced oxygen is for the minimized number of trays given in 4.4.

$$\frac{6052kW}{0.211kmol/s \bullet 0.956kmol_{O_2}/kmol \bullet 32.00kg_{O_2}/kmol_{O_2} \bullet 3600s/h} = 0.260kW/kg_{O_2} \quad (4.4)$$

The energy consumption per kilogram of pure oxygen is increased with about 2 percent.

Figure 4.3 shows the separation factor for the high pressure column with 11 trays.
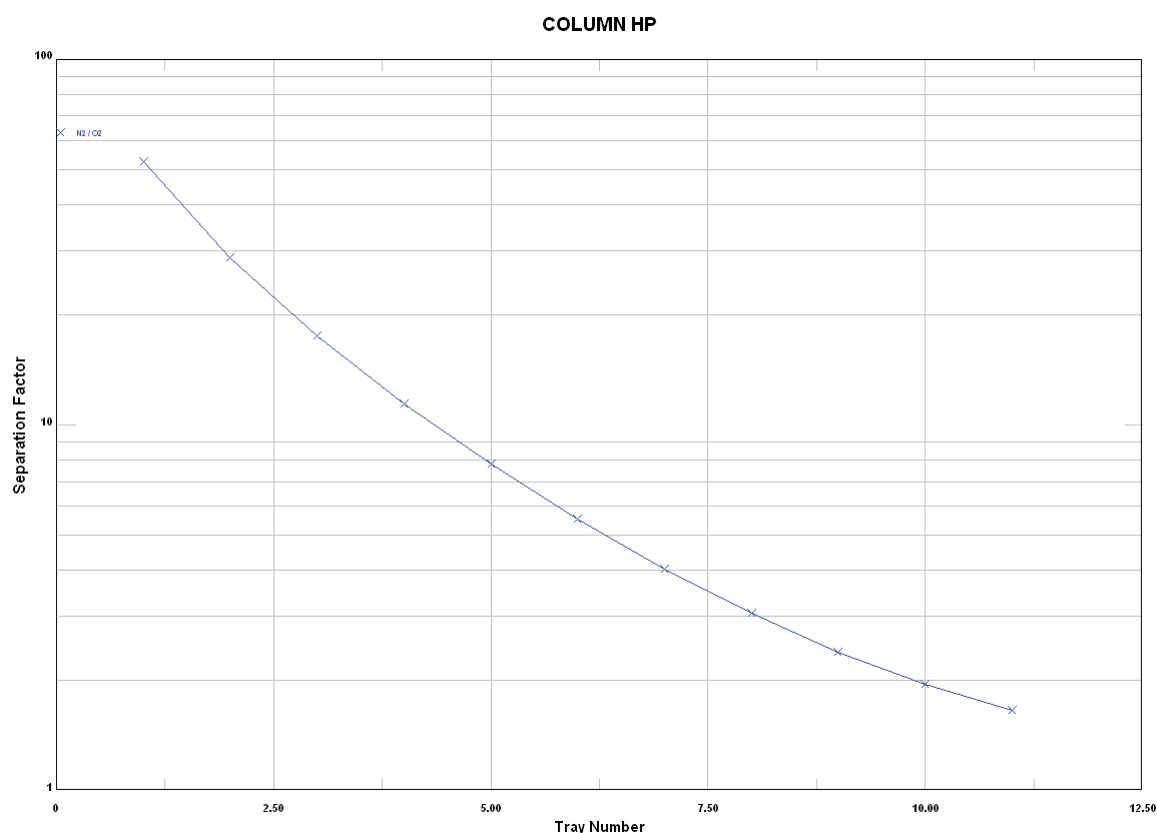
Figure 4.3. Separation factor for high pressure column with 11 trays.

If figure 4.3 is compared with figure 3.3 in *3.1.2.4 High pressure column,* it can be seen that the separation factor in both cases is placed between 1 and 2 for the last tray. Figure 4.3 is a little closer to 2 than figure 3.3 because of the small decrease in nitrogen purity. But the nitrogen purity is still at an acceptable level.

The number of trays in the LP column is as mentioned adjusted after the duty in the combined condenser and reboiler which is dependent on the number of trays in the HP column. A figure of separation factor for the LP column with 16 trays is shown in figure 4.4.
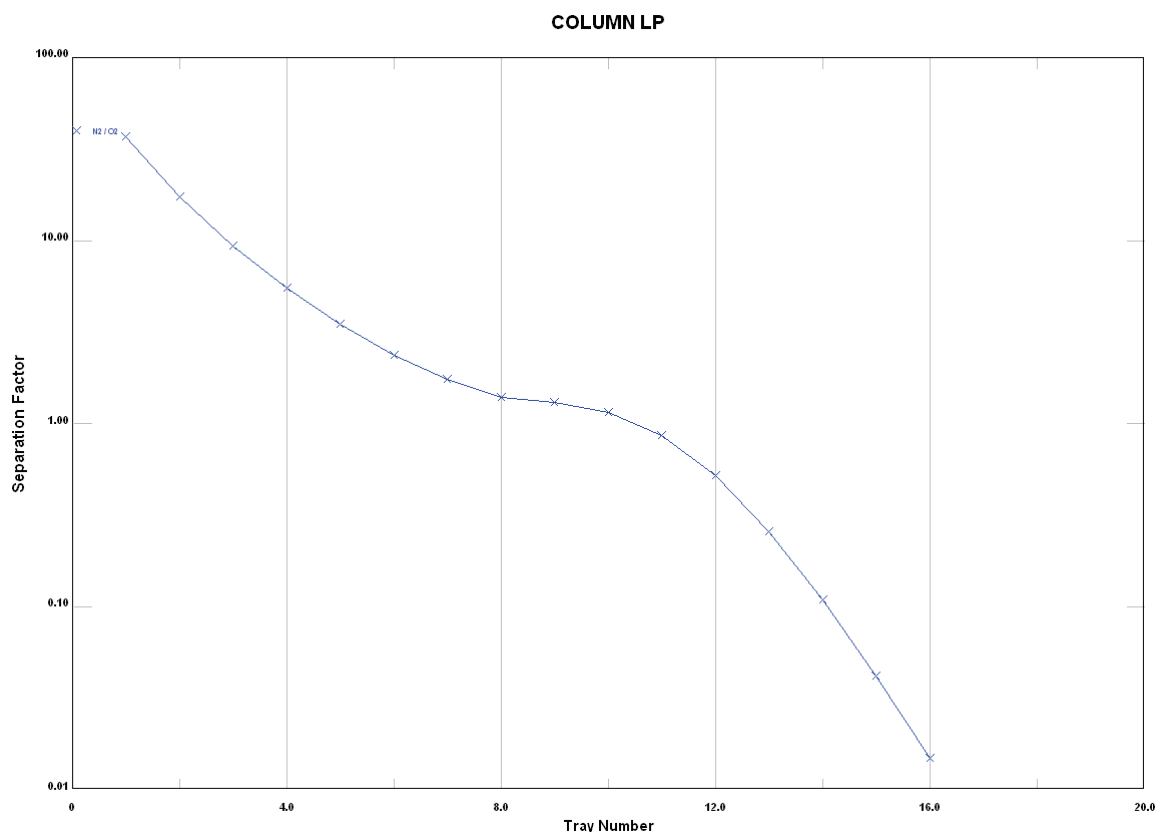
Figure 4.4. Separation factor for low pressure column with 16 trays.

With concern to purity level of the oxygen out of the plant, OX9, the low pressure column could in fact have fewer trays. Since the duty of the modeled reboiler has to be equal to the condenser, the number of trays is higher than necessary to achieve the wanted oxygen purity. The oxygen purity is by this maintained at 95.6 percent.

A minimization of the number of trays leads as mentioned to a 2 percent increase in energy consumption per kg oxygen and to maintain the consumption of 0.254 per kg the there is a need of 24 trays in the HP column and 32 Trays in the LP column. This is probably near optimal solution when minimization of energy consumption is taken into account together with minimization of number of trays.

4.1.1.5   Argon considerations

Argon has its boiling point between oxygen and nitrogen. It is assumed that the boiling point of oxygen, nitrogen and argon is changed approximately linearly for different pressures

compared to each other. It is also assumed that the boiling points can decide the distribution of argon between OX9 and NI8 and this is then given by equation 4.5.

$$\frac{T_{boiling,nitrogen,1atm} - T_{boiling,oxygen,1atm}}{T_{boiling,nitrogen,1atm} - T_{boiling,argon,1atm}} = \frac{77.4K - 87.3K}{77.4K - 90.3K} = 0.77 \tag{4.5}$$

From this calculation the oxygen stream OX9 should contain 77% of the argon in the air.

The amount of argon in the oxygen stream found in PRO/II can be calculated from table 4.1.

$$\frac{(0.216 \cdot 0.033)}{(0.216 \cdot 0.033) + (0.774 \cdot 0.002)} = 0.82 \tag{4.6}$$

The modeled distribution of argon between the OX9 and NI8 of 82 to 18 is close to the hypothesis and support the validity of the model.

4.1.1.6   Overall GOX considerations

It is possible to lower the energy consumption by minimizing ΔT in the combined condenser reboiler. But by doing this the purity of the nitrogen stream out, NI8, is reduced. Therefore, both the purity and ΔT has to be kept at an acceptable level.

The number of trays also has an impact on the purity. An optimization concerning minimization of number of trays, keeping ΔT and the purity level at acceptable levels and minimize the energy consumption must be done.

Also the pressure loss in the columns has impact on the purity level and compression work. Pressure loss in the HP column has direct impact on the compression work. Pressure loss in the LP column has impact on the temperature difference in the combined condenser and reboiler which has impact on compressor work through the HP column.

There are many free variables and there might be different solutions leading equal answers. Another important point of view is that many of the decisions that need to be made are

concerning investment costs versus operating costs. To find a specific optimal solution demands an economic analysis concerning both equipment and energy expenses.

For further GOX calculations a near optimal solution found by iterations and the small adjustments discussed in the previous sections, is used. Equation 4.7 gives the energy consumption per kilogram oxygen produced and table 4.6 gives the key numbers in the model. All stream and compressor properties are given in Appendix J.

$$\frac{5673 kW}{0.216 kmol/s \bullet 0.956 kmol_{O_2}/kmol \bullet 32.00 kg_{O_2}/kmol_{O_2} \bullet 3600 s/h} = 0.238 kW/kg_{O_2} \quad (4.7)$$

Table 4.6. Key GOX numbers.

Air feed to ASU	Pressure		1 bar
	Temperature		298 K
	Flowrate		1 kmol/s
	Composition	O_2	77.3 %
		N_2	20.7 %
		AR	0.9 %
		H_2O	1.0 %
		CO_2	0.0 %
Compressor	Number of compressors		4
	Total work, 1 kmol/s moist air		5673 kW
	Pressure raise		5.6 bar
	Polytrophic compressor efficiency		85 %
Main heat exchanger and molecular sieves	Total pressure loss		0.3 bar
HP column	Number of trays		24
	Top pressure		5.1 bar
	Bottom pressure		5.3 bar
	Pressure loss trough column		0.2 bar
LP column	Number of trays		32
	Top pressure		1.1 bar
	Bottom pressure		1.4 bar
	Pressure loss trough column		0.4 bar
Combined condenser and reboiler	Condenser temperature		94.37 K
	Condenser pressure		5.1 bar
	Reboiler temperature		92.93 K
	Reboiler pressure		1.4 bar
	Temperature difference		1.44 K
	Duty transferred		2510 kW
Oxygen out of ASU	Purity of oxygen		95.6 %
	Pressure		1.4 bar
	Temperature		297 K
	Flowrate		0.216 kmol/s
	Composition	O_2	95.6 %
		N_2	1.1 %
		AR	3.3 %
Nitrogen out of ASU	Purity of nitrogen		99.6 %
	Pressure		1.1 bar
	Temperature		291 K
	Flowrate		0.774 kmol/s
	Composition	O_2	0.2 %
		N_2	99.6 %
		AR	0.2 %
Waste out of ASU	Flowrate		0.01 kmol/s
	Composition	H_2O	97.1 %
		CO_2	2.9 %
Energy consumption	**Per kg produced oxygen**		**0.238 kW/kg$_{O2}$**

Figure 4.5 shows the PRO/II model of the final model.
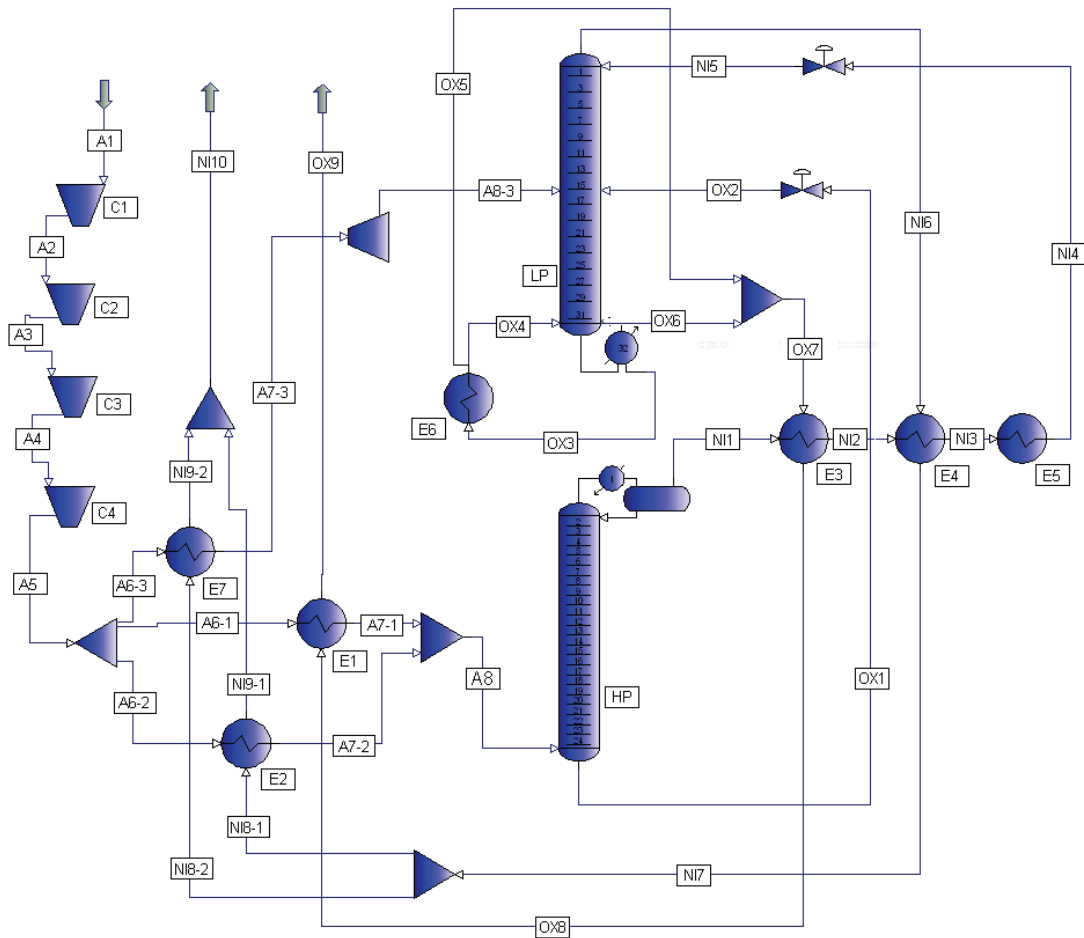
Figure 4.5. Final GOX model.

An influential parameter is the polytrophic compressor efficiency. This factor is in the simulations set to 85%. Other may operate with different efficiency and this has major impacts on the energy consumption per kilogram pure oxygen produced. For examples is some literature operating with 90% percent polytrophic efficiency [6], while commercial companies sometimes operate with lower compressor efficiency.

If the model is changed to have a polytrophic compressor efficiency of 90% the energy consumption per kilogram oxygen is reduced to $0.224 kWh/kg_{O2}$. A reduction of compressor efficiency to 82% leads to an increase in consumption to $0.242 kWh/kg_{O2}$.

4.1.2   *Liquid oxygen*

The LOX model is as mentioned in *3.1.3 Liquid oxygen,* an expansion of the GOX model. The energy consumption per kilogram oxygen produced is not as straight forward presented as for a GOX plant. The GOX model has an energy consumption given for oxygen at about ambient conditions. The point of a LOX plant is to deliver oxygen out of ASU at high pressure and to compare direct with a GOX model is unfair. To be able to compare, the oxygen flow from the GOX model needs to be compressed to an equal pressure to the LOX model.

The chosen pressure level is adjusted to the pressure wanted in the gasifier. This pressure is set to 42bar. To compare the models, the pump in the LOX model and the oxygen compressor in the end of the GOX model, are both set to have an outcome pressure of 42bar.

The LOX plant has initially the same specifications as the initial GOX plant. 40 trays in both HP and LP column and the same pressure levels and losses. The LOX model developed is very sensitive and small adjustments or regulations may give convergence problems. The developed LOX model is therefore compared with the GOX plant with equal specifications and if the results from the LOX look good, the model is optimized.

With equal specifications, the outcome of the two models is also quite similar. The purity and amount of oxygen and nitrogen is in fact exact equal. Stream specifications for all streams in the LOX model are given in Appendix K and a figure of the model is shown in *3.1.3 Liquid oxygen.*

Because of equal amounts and purities in the two models, compression work is the only factor needed to be compared. The GOX model has compression work in the main heat exchanger and in the oxygen compressor. To model an as comparable model as possible, the oxygen compressor is modeled in two steps. This is done to have comparable lifting heights in the booster air compressor in the LOX model and the oxygen compressor in the GOX model.

The LOX model has compression work in the main heat exchanger, the mentioned booster air compressor and a small pump work in the oxygen pump. The compressor information for the two models is presented in table 4.7 and 4.8.

Table 4.7. Compression work initial GOX model.

Compressor Name		C1	C2	C3	C4	C5	C6
		Main	Main	Main	Main	Air	Air
Pressure	bar	1.600	2.500	4.000	6.430	6.300	42.000
Temperature	K	348.940	348.389	351.332	351.905	476.891	554.210
Head	m	5224.165	5166.875	5468.312	5525.645	16895.041	24386.836
Actual Work	kW	1469.220	1453.108	1537.882	1554.007	1153.192	1663.127
Isentropic coef., k		1.401	1.402	1.404	1.407	1.396	1.406

Table 4.8. Compression work initial LOX model.

Compressor Name		C1	C2	C3	C4	C5	P1
		Main	Main	Main	Main	Booster	Pump
Pressure	bar	1.600	2.500	4.000	6.430	40.000	42.000
Temperature	K	348.940	348.193	351.332	351.905	550.815	n/a
Head	m	5224.165	5163.930	5468.312	5525.645	26404.031	200.084
Actual Work	kW	1469.220	1745.669	1848.566	1867.947	2250.226	15.146
Isentropic coef., k		1.401	1.402	1.404	1.407	1.417	n/a

This gives a total work demand of 8831 kW for the GOX model and 9197 kW for the LOX model. This equals a 4 percent higher energy demand in the LOX model than the GOX model.

The LOX production method described in *2.1.2.10 Liquid oxygen* in the theoretical background feeds the booster compressed air to the high pressure column. This is not possible in the model developed in this report. The model developed here has a need of cooling in the subcooler, in the nitrogen stream between the HP and LP column. As mentioned in *3.1.3.2 Minimum temperature approach problems*, the booster compressed air is not cold enough to cool the nitrogen stream when choked to HP pressure level. Therefore it has to be choked lower than HP pressure and a need of recompression occurs. This leads to increased work in the main compressor making the LOX model more energy demanding than the GOX model.

Due to higher energy demand in the LOX model compared to the initial GOX model, further optimization of the LOX model is not prioritized. The solution of 0.238 kWh per kilogram of produced oxygen presented in *4.1.1.6 Overall GOX considerations* is used in further calculations.

4.2 Gasification Island

4.2.1 Introduction

Calculations and modeling on gasification of three different coals are described in the method part. Here the results will be presented and discussed. Results from MatLab calculations, PRO/II and GTPRO simulations and other calculations are presented in the upcoming chapters.

4.2.2 MatLab calculations

The MatLab program calculates the equilibrium conditions based on elements and not as molecules. This will give other molar fractions since H_2, O_2 and N_2 have other molecular weights than H, O and N. The compositions of the three coals as elements are presented in table 4.9. The amount of O_2 and H_2O for the gasification process is the same as the amounts found from the PRO/II simulations. These numbers are discussed closer in *4.2.3 Pro/II simulations*.

Table 4.9. Molar fractions for MatLab calculations.

Coal		Mol Fraction						Reactants	
Region	Classification	C	H	O	N	S	H_2O	O_2	H_2O
Rhein	Browncoal	0.569	0.126	0.041	0.001	0.002	0.261	0.179	0.000
Datung	Bituminous	0.597	0.346	0.050	0.005	0.002	0.000	0.280	0.130
Ruhr	Anthracite	0.679	0.296	0.014	0.009	0.002	0.000	0.300	0.200

It should be noted that for the Browncoal the H_2O is included in the total composition. This indicates that it is a model of a wet slurry coal feed.

The feed from table 4.9 calculated with the MatLab equilibrium calculator give the following molar fractions of syngas. These calculations only show the CO, CO_2, H_2 and H_2O because of the mentioned convergence problems using all the elements. It is however the most relevant gasses that is presented here.

Table 4.10. Syngas composition for different coals calculated in MatLab.

Coal		Browncoal	Browncoal	Bituminous	Bituminous	Anthracite	Anthracite
Temperature	C	1481	1481	1572	1572	1233	1233
Pressure	Bar	42	42	42	42	42	42
syngas composition		Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction
CO		0.601	0.643	0.601	0.666	0.600	0.645
CO_2		0.037	0.040	0.062	0.069	0.061	0.066
H_2		0.298	0.319	0.239	0.265	0.269	0.289
H_2O		0.065	0.000	0.098	0.000	0.070	0.000

The temperatures here are equivalent with the ones from the PRO/II simulations discussed in the next chapter. The literature handles with gas analysis on dry basis. Therefore the water is removed to get comparable results. The shaded columns show the molar fractions on dry basis. To calculate the dry gas composition the water content in the syngas is removed. An example of this calculation is shown for CO and H_2 for the Browncoal in table 4.10.

$$y_{co_{dry}} = \frac{y_{co}}{1 - y_{H_2O}} = \frac{0.601}{1 - 0.065} = 0.643 \qquad (4.8)$$

$$y_{H_{2dry}} = \frac{y_{H_2}}{1 - y_{H_2O}} = \frac{0.298}{1 - 0.065} = 0.319 \qquad (4.9)$$

4.2.3   PRO/II simulations

The results from the PRO/II simulations on three different coals will be presented here. Finding the oxygen (and steam) amount and to get a syngas composition close to the one found in literature is the main goal for these calculations.

4.2.3.1   Gasification of Browncoal

Table 4.11 gives the different flow rates from the PRO/II calculation of the Browncoal. The coal contains considerable amount of water and the only gasification agent is therefore the oxygen. The column to the right is showing the syngas at normal state. This is calculated using the method presented in *3.2.4.2 Modeling Gasification Island*, and is only interesting

for comparing with given literature. A heat exchanger that normalizes the product gas will not be included in a gasification plant and is only used as a calculation tool.

Table 4.11. Different flow rates for Browncoal gasification.

		Coal	Oxygen	Syngas	Nm^3 Syngas
Temperature	C	25.000	25.000	1480.743	15.000
Pressure	Bar	42.000	42.000	41.600	1.013
Rate	kmol/s	1.000	0.179	0.931	0.931
	kg/s	12.692	5.728	18.420	18.420
Actual Rate	m^3/s	0.173	0.104	3.276	17.359
Standard Vapor Rate	m^3/s	6.460	4.012	20.862	16.452

The amounts of oxygen (and steam) were found doing iteration between syngas composition, temperature and amount of the different feed. The results from this will be presented here.

Nm^3 syngas / ton maf coal

The rate of produced syngas can be calculated from table 4.11 and table 4.12. Syngas is defined as CO and H$_2$ and therefore will only these substances be included in the calculation. From Table 4.12 the syngas fraction can be found, $0.502CO + 0.246H_2 = 0.748$syngas. The normalized flow is found from table 4.11 to be 17.359 and the volume flow of syngas at normal conditions then becomes $17.359 \cdot 0.748 = 12.985$ Nm^3. The mass flow is taken directly from Table 4.11, 12.692 kg/s. These numbers are then adjusted to get the rate at Nm^3/ton form.

$$\frac{12.985 \left[Nm^3 \right]}{12.692 \left[kg \right]} \cdot 1000 \left[\frac{kg}{ton} \right] = 1023 \left[\frac{Nm^3}{ton} \right] \tag{4.10}$$

Nm^3 O$_2$ / Nm^3 Syngas

The consumption of oxygen per m^3 syngas can be calculated directly from the table using the standard vapor rate since the correlation between standard and normal condition is the same for O$_2$ and syngas.

$$\frac{4.012 \left[Sm^3 \right]}{0.748 \cdot 16.452 \left[Sm^3 \right]} = 0.326 \tag{4.11}$$

This number is then similar to Nm^3 over Nm^3 syngas and is therefore comparable with the values from table 3.11 in *3.2.4.1 Introduction*.

The dry gas fractions are shown as the shaded column in table 4.12, these values are calculated using the principles from equation 4.8 and 4.9.

Table 4.12. Syngas composition and O_2 consumption for Browncoal.

		Coal	Oxygen	Syngas	Nm^3 syngas	Nm^3 dry syngas
Temperature	C	25.000	25.000	1480.743	15.000	15.000
Pressure	bar	42.000	42.000	41.600	1.013	1.013
Flowrate	kmol/s	1.000	0.179	0.931	0.931	0.722
Composition						
C		0.487	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.502	0.502	0.648
CO_2		0.000	0.000	0.021	0.021	0.027
O_2		0.071	1.000	0.002	0.002	0.002
H_2		0.215	0.000	0.246	0.246	0.317
H_2O		0.223	0.000	0.225	0.225	0.000
CH_4		0.000	0.000	0.000	0.000	0.000
N_2		0.002	0.000	0.002	0.002	0.003
NO		0.000	0.000	0.000	0.000	0.000
S		0.002	0.000	0.000	0.000	0.000
SO_2		0.000	0.000	0.002	0.002	0.003
H_2S		0.000	0.000	0.000	0.000	0.000

4.2.3.2　Gasification of Bituminous

Gasification of Bituminous (and Anthracite) also includes steam as an input factor. Table 4.13 shows the flow rate of the oxygen, the steam and the syngas printed from PRO/II. The column to the right is the normalized flow rate of the syngas. These numbers are a result of trial and failure among oxygen/steam feed to reach level similar to the literature.

Table 4.13. Different flow rates for Bituminous gasification.

		Coal	Steam	Oxygen	Syngas	Nm^3 Syngas
Temperature	C	25.000	255.000	25.000	1571.858	15.000
Pressure	bar	42.000	42.000	42.000	41.600	1.013
Rate	kmol/s	1.000	0.130	0.280	1.097	1.097
	Kg/s	10.453	2.342	8.960	21.755	21.755
Actual Rate	m^3/s	0.158	0.113	0.162	4.069	25.940
Standard Vapor Rate	m^3/s	5.884	2.914	6.276	24.583	24.582

The results from table 4.13 can be used to calculate the production rate and the consumption rate of oxygen/steam as described in *3.2.4.2 Modeling Gasification Islands*.

Nm³ syngas / ton maf coal

Table 4.13 shows that the given reaction give1.097kmol product gas at a temperature 1571.9˚C and at a pressure of 41.6bar. Normalizing this amount gives a rate of 25.94kmol product gas. From table 4.14 the syngas fraction ca be found as 0.669CO+0.311H$_2$=0.98syngas, and the volume of syngas then becomes 25.94·0.98=25.42Nm³. Produced syngas per ton coal can then be calculated.

$$\frac{25.42\left[Nm^3\right]}{10.45\left[kg\right]}\cdot1000\left[\frac{kg}{ton}\right]=2433\left[\frac{Nm^3}{ton}\right] \tag{4.12}$$

Nm³ O₂ / Nm³ Syngas

The consumption of oxygen per m³ syngas can be calculated directly from table 4.13 using the standard vapor rate since the correlation between standard and normal condition is the same for O$_2$ and syngas.

$$\frac{6.276\left[Sm^3\right]}{0.980\cdot24.582\left[Sm^3\right]}=0.261 \tag{4.13}$$

Kg steam / Nm³ syngas

The consumption rate of steam is measured in mass and not as a volume. This is because steam at normal condition is liquid water. The mass flow of steam is from table 4.13 known as 2.342kg/s and the normalized amount of syngas is still 25.46Nm³. The steam to syngas rate is then given by equation 4.14.

$$\frac{2.342\left[kg\right]}{25.42\left[Nm^3\right]}=0.092 \tag{4.14}$$

With the given amount of steam and oxygen the composition of the produced gas can be studied in table 4.14.

Table 4.14. Syngas composition and O_2/steam consumption for Bitumimous.

		Coal	Steam	Oxygen	Syngas	Nm^3 syngas	Nm^3 dry syngas
Temperature	C	25.000	255.000	25.000	1571.583	15.000	15.000
Pressure	bar	42.000	42.000	42.000	41.600	1.013	1.013
Flowrate	kmol/s	1.000	0.130	0.280	1.097	1.097	1.082
Composition							
C		0.735	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.669	0.669	0.678
CO$_2$		0.000	0.000	0.000	0.001	0.001	0.001
O$_2$		0.031	0.000	1.000	0.000	0.000	0.000
H$_2$		0.228	0.000	0.000	0.311	0.311	0.315
H$_2$O		0.000	1.000	0.000	0.014	0.014	0.000
CH$_4$		0.000	0.000	0.000	0.000	0.000	0.000
N$_2$		0.003	0.000	0.000	0.003	0.003	0.003
NO		0.000	0.000	0.000	0.000	0.000	0.000
S		0.003	0.000	0.000	0.000	0.000	0.000
SO$_2$		0.000	0.000	0.000	0.000	0.000	0.000
H$_2$S		0.000	0.000	0.000	0.002	0.002	0.002

The syngas produced from the Bituminous is the basis for the rest of the model including water gas shift reforming, CO_2 removing and the power cycle. This is a high ranked coal typical used in gasification processes.

4.2.3.3   Gasification of Anthracite

The same principle as for the Bituminous coal is used doing calculations on the Anthracite coal from Ruhr.

Table 4.15. Different flow rates for Anthracite gasification.

		Coal	Steam	Oxygen	Syngas	Nm^3 Syngas
Temperature	C	25.000	255.000	25.000	1233.572	15.000
Pressure	bar	42.000	42.000	42.000	41.600	1.013
Rate	kmol/s	1.000	0.200	0.300	1.190	1.190
	kg/s	10.441	3.603	9.600	23.644	23.644
Actual Rate	m^3/s	0.120	0.173	0.173	3.610	28.136
Standard Vapor Rate	m^3/s	4.478	4.483	6.724	26.663	26.663

From table 4.16 the syngas fraction can be found, 0.668CO+0.310H$_2$=0.978 syngas. The volume flow at normal conditions then becomes 28.136·0.978=27.517Nm^3. Produced syngas per ton of coal is calculated as before.

$$\frac{27.52\left[Nm^3\right]}{10.44\left[kg\right]} \cdot 1000\left[\frac{kg}{ton}\right] = 2635\left[\frac{Nm^3}{ton}\right] \tag{4.15}$$

The same procedure as for Bituminous is used to find the oxygen rate and the steam rate. This gives is given by the following equations.

$$\frac{6.724\left[Sm^3\right]}{0.978 \cdot 26.663\left[Sm^3\right]} = 0.258 \tag{4.16}$$

$$\frac{3.603\left[kg\right]}{27.52\left[Nm^3\right]} = 0.131 \tag{4.17}$$

The given amounts of O_2 and steam give the following results.

Table 4.16. Syngas composition and O_2/steam consumption for Anthracite.

		Coal	Steam	Oxygen	Syngas	Nm^3 syngas	Nm^3 dry syngas
Temperature	C	25.000	255.000	25.000	1233.572	15.000	15.000
Pressure	bar	42.000	42.000	42.000	31.600	1.013	1.013
Flowrate	kmol/s	1.000	0.200	0.300	1.190	1.190	1.174
Composition							
C		0.798	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.668	0.668	0.677
CO_2		0.000	0.000	0.000	0.002	0.002	0.002
O_2		0.008	0.000	1.000	0.000	0.000	0.000
H_2		0.186	0.000	0.000	0.310	0.310	0.314
H_2O		0.000	1.000	0.000	0.013	0.013	0.000
CH_4		0.000	0.000	0.000	0.000	0.000	0.000
N_2		0.005	0.000	0.000	0.004	0.004	0.004
NO		0.000	0.000	0.000	0.000	0.000	0.000
S		0.002	0.000	0.000	0.000	0.000	0.000
SO_2		0.000	0.000	0.000	0.000	0.000	0.000
H_2S		0.000	0.000	0.000	0.002	0.002	0.002

4.2.3.4   Comparison

The calculated results can be summarized in table 4.17 which corresponds to the values in table 3.11 in *3.2.4.1 Introduction*.

Table 4.17. Summarize of the calculated amounts.

Coal		Amount of reactants and products		
Region	Classification	Nm^3 syngas/ ton maf coal	Nm^3 O$_2$/ Nm^3 syngas	kg steam/ Nm^3 syngas
Rhein	Browncoal	1024	0.326	0
Datung	Bituminous	2433	0.261	0.092
Ruhr	Anthracite	2635	0.258	0.131

Table 4.17 shows that gasification of Browncoal requires relative high oxygen consumption and produces a relative small amount of syngas per ton of coal. That supports the theory that entrained flow gasification for IGCC application is best suitable for high ranked coal. Distillation of oxygen from air is an energy demanding procedure that contributes considerable to the overall efficiency. The air separation is discussed in detail in *4.1. Air Separation Island*.

From table 4.17 it can be read that the production rate of syngas per mass coal is higher than the numbers from the literature. The main reason for this is that the gasification models made here do not take care of ash and other substances. Therefore the performance capacity for this facility is higher than it will be in real life. For Bituminous and Anthracite the tendency is quite the same. The relative deviation from literature for Bituminous is given by equation 4.18.

$$\frac{Calc - Theo}{Theo} = \frac{2433 - 2060}{2433} = 0.153 \tag{4.18}$$

Similar calculation for Anthracite gives 0.161 which provide proves a relation here for the Dry-Fed gasifier. It is not surprising when the coal types are closed to each other in ranking and also in oxygen and steam consumption. The results of syngas composition for each coal can be summarized in table 4.18**.** This table corresponds to table 3.10 in *3.2.4.1 Introduction***.**

Table 4.18 summarize of the syngas compositions.

Coal		Product Gas Mol Fraction (dry)					
Region	Classification	CO	H$_2$	CO$_2$	N$_2$	A	H$_2$S
Rhein	Browncoal	0.648	0.317	0.027	0.003	0.000	0.000
Datung	Bituminous	0.678	0.315	0.001	0.003	0.000	0.002
Ruhr	Anthracite	0.677	0.314	0.002	0.004	0.000	0.002

The fractions differ a little. The fact that ash is not included will play a role. If ash was a part of the mixture the fractions of CO and H_2 would have decreased and brought nearer to the values in table 3.10. All in all the models give workable results compared to expected values. The fact that the production of syngas exceeds the values from the literature will affect the overall efficiency positively. Compared to real life a larger amount of coal will be required to produce the wanted amount of syngas. This will give a higher total Q_{in} (LHV) and again a lower net efficiency according to equation 2.56.

4.2.4   Equilibrium calculator

The online equilibrium calculator can handle coal as a mixture of C, H_2, O_2, S and N_2 (gasses) and as pure elements in the same way as the MatLab program discussed in *4.2.2 MatLab calculations*. There are run calculations on both scenarios.

4.2.4.1   Coal fed as a mixture of elements and molecules

Table 4.18 shows the equilibrium composition when the coal wis fed as a mixture and the hydrogen, oxygen and nitrogen are on molecular form. The carbon and sulfur are fed as pure elements.

Table 4.19. Syngas composition, coal fed as elements and molecules.

Coal		Browncoal	Browncoal	Bituminous	Bituminous	Anthracite	Anthracite
Temperature	C	1481	1481	1572	1572	1233	1233
Pressure	Bar	42	42	42	42	42	42
syngas composition		Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction
C		0.000	0.000	0.000	0.000	0.000	0.000
CO		0.499	0.539	0.686	0.686	0.669	0.678
CO_2		0.026	0.028	0.000	0.000	0.007	0.007
O_2		0.000	0.000	0.000	0.000	0.000	0.000
H_2		0.395	0.427	0.263	0.263	0.295	0.295
H_2O		0.075	0.000	0.000	0.000	0.008	0.000
CH_4		0.025	0.027	0.045	0.045	0.014	0.014
N_2		0.003	0.003	0.003	0.003	0.004	0.004
NO		0.000	0.000	0.000	0.000	0.000	0.000
S		0.000	0.000	0.000	0.000	0.000	0.000
SO_2		0.000	0.000	0.000	0.000	0.000	0.000
H_2S		0.002	0.002	0.003	0.003	0.002	0.002

The results from table 4.18 show a relation between the PRO/II calculations and the calculator. The case of Anthracite and Bituminous give much the same values. The main deviation is that the online calculator gives an amount of CH_4 in the products which again decreases the amount of H_2 since 1mole of CH_4 contains 1C and 4H. In PRO/II these substances are distributed among CO, CO_2 and H_2 and therefore it will give a higher fraction of H_2 due to the molar balance. CH_4 is favored by low temperature and this is a likely explanation of the differences between the two calculations. In PRO/II the temperature is a function of the fed and will vary during the gasification process, while the calculator does calculation for given temperatures. For the special case of Browncoal the differences can also be a result of the feeding of water. For the Dry feed gasifiers the water is fed separately at 255˚C while the Slurry Fed gets the water part included in the coal feed at lower temperature. In the calculator there is no feeding procedure that differs if the water is a part of the coal or a separate reactant.

4.2.4.2   Coal fed as elements only

Table 4.20 gives the results from a calculation with pure elements, which means for example that the hydrogen part of the feed is defined as H instead of H_2. That gives different molar fractions in the feed compared to the case where the feed is presented as both elements and molecules. An example of a transcript from the online chemical calculator is given in Appendix L.

Table 4.20. Syngas composition, coal fed as elements only.

Coal		Browncoal	Browncoal	Bituminous	Bituminous	Anthracite	Anthracite
Temperature	C	1481	1481	1572	1572	1233	1233
Pressure	bar	42	42	42	42	42	42
syngas composition		Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction	Mole fraction	Dry mole fraction
C		0.000	0.000	0.000	0.000	0.000	0.000
CO		0.605	0.642	0.599	0.664	0.602	0.645
CO_2		0.032	0.034	0.062	0.069	0.058	0.062
O_2		0.000	0.000	0.000	0.000	0.000	0.000
H_2		0.301	0.320	0.236	0.262	0.265	0.284
H_2O		0.058	0.000	0.098	0.000	0.067	0.000
CH_4		0.000	0.000	0.000	0.000	0.001	0.001
N_2		0.002	0.002	0.003	0.003	0.004	0.004
NO		0.000	0.000	0.000	0.000	0.000	0.000
S		0.000	0.000	0.000	0.000	0.000	0.000
SO_2		0.000	0.000	0.000	0.000	0.000	0.000
H_2S		0.002	0.002	0.002	0.002	0.002	0.002

The results from table 4.20 are quite similar to the results from table 4.19. The main trend is that the last one produces more CO_2 and therefore less CO. Also here the Browncoal values differ more than the other ones. But here they are closer to the values from the PRO/II simulation. Anyway the results all in all give satisfactory results and it indicates that the PRO/II model is useful. Compared with the MatLab program the results are very close. This proves that the MatLab calculator is useful for simplified coal compositions.

4.2.5   Water shift reforming

4.2.5.1   Water gas shift reactor

Three coals are studied. For further simulations and calculations only one coal is used. This is the Bituminous. The syngas from this specific coal is used as feed for the water shift reactor. There are modeled two stages of the shift reactor. Water steam is added to increase the H_2 production. The amount of water and the compositions before, between and after the whole process is presented in table 4.21.

Table 4.21. Molar compositions for different stages.

Stream Name		Cooled syngas	Steam	Intermediate gas	H₂-rich gas	Dry-H₂ rich gas
Phase		Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	C	250.000	255.000	498.535	294.105	36.670
Pressure	bar	41.400	41.400	41.000	40.400	40.200
Flowrate	kmol/s	1.097	1.07	2.167	2.167	1.772
Composition						
C		0.000	0.000	0.000	0.000	0.000
CO		0.669	0.000	0.085	0.020	0.024
CO₂		0.001	0.000	0.254	0.319	0.390
O₂		0.000	0.000	0.000	0.000	0.000
H₂		0.311	0.000	0.411	0.476	0.582
H₂O		0.014	1.000	0.247	0.182	0.000
CH₄		0.000	0.000	0.000	0.000	0.000
N₂		0.003	0.000	0.002	0.002	0.002
NO		0.000	0.000	0.000	0.000	0.000
S		0.000	0.000	0.000	0.000	0.000
SO₂		0.000	0.000	0.000	0.000	0.000
H₂S		0.002	0.000	0.001	0.001	0.001

The product gas from the first stage has a temperature of 499°C and this is cooled to 225°C before the second stage. This is called the intermediate gas inn the table. The column to the left shows the composition after the water has been removed. In the first stage there is fed 1.07kmol of steam for this amount of syngas. It should be kept in mind that these numbers are valid for a coal feed of 1kmol. When it comes to the total plant the amounts will be adjusted to fit the turbine. The ratio between fed steam and fed CO will be independent of the coal feed and is for this shift reactor given in equation 4.19.

$$\frac{H_2O}{CO} = \frac{1.097 \cdot 0.014 + 1.070 \cdot 1.000}{1.097 \cdot 0.669} = 1.479 \qquad (4.19)$$

Compared to literature [21] this is a realistic value. The ratio may be as high as 2, however this will give more H_2O in the product gas that has to be condensed before the CO_2 capture unit anyway. There are also limitations according to the fraction of water in the product gas. It should not exceed 0.2 [10]. In addition is a CO fraction of 0.02 a realistic value. Addition of more steam is also an energy requiring process so this is seen as a satisfactory result.

With these conditions one mole of coal will give 2.167*0.427=1.031kmol of H_2. The 2 % of CO has also heating values and can be fed to a turbine. Normally is H_2O an excellent diluter, but in this case will the combustion process form a relatively high amount of water so the total amount will be too high for the turbine. The high amount of CO_2 makes it relatively easy to remove it. A molar fraction of 0.390 after the water removing and a total pressure of 40.2bar gives a partial pressure of CO_2 of 15.68bar. This is advantageous for the removing process. The N_2 is low and anyway a good substance to feed together with the H_2 rich fuel. More N_2 will be fed after the CO_2 capture unit before the combustion chamber in the gas turbine.

4.2.5.2   Integrating the gasification and water shift

The temperature of the syngas can be reduced by adding more water into the gasifier. This again will give more H_2O in the syngas and reduce the additional steam demand in the shift reactor. Allocating the steam/water in other ways gives no considerable changes. The composition from table 4.21 is therefore sent further to the CO_2 capture unit before it is diluted with nitrogen and fed to the power cycle.

The chosen coal going through the gasifier and two stages of water shift reactors generates heat in all processes. This is because the overall reactions are more exothermic than endothermic. This can be expressed in the term of cold gas efficiency. The heating value for the coal using equation 3.23 is given in equation 4.20.

$$LHV_{coal} = 0.736 \cdot 393520 + 0.228 \cdot 241820 + 0.003 \cdot 296800 = 345656 \left[\frac{kJ}{kmol} \right] \qquad (4.20)$$

The bituminous has a molar weight of 10.455kg/kmol and the LHV becomes on mass basis 345956/10.455=33090kJ/kg. This is much closed to the tabulated value from table 2.3 in *2.2.1.1 composition* which operates with a LHV of 33400kJ/kg for Bituminous. LHV for the CO and H_2 mix is then given by equation 4.21.

$$LHV_{syngas} = 1.097 \cdot [0.669 \cdot 282990 + 0.311 \cdot 241820] = 290185 \left[\frac{kJ}{kmol} \right] \qquad (4.21)$$

This gives a CGE of:

$$CGE = \frac{290185}{345656} = 0.840 \tag{4.22}$$

This value corresponds to the literature. It is stated that a gasification process requires a CGE of at least 0.78 to make IGCC attractive [6].

The LHV for the H_2 rich fuel is loosing some more heating value and for this case it is given by equation 4.23.

$$LHV_{H_2 rich} = 1.967 \cdot [0.02 \cdot 282990 + 0.527 \cdot 241820] = 261806 \left[\frac{kJ}{kmol} \right] \tag{4.23}$$

This indicates that there is a loss in heating values through the process. In an IGCC some of the heat that is released can be utilized in other processes and improve efficiency. This will be discussed more in *4.4.2.2 Adding steam to the steam turbine*.

4.3 Acid Gas Removal

4.3.1 Considerations

As mentioned in *3.3.2 CO₂ capture unit*, there is not done any modelling on the CO_2 scrubber. The composition after the scrubber is calculated in Excel and is shown in table 3.14 in *3.3.2 CO₂ capture unit*.

There will always be pressure losses in a process. The pressure of the fuel gas in to the CO_2 capture unit is at 40.2bar. After acid gas removal the next step is to dilute with nitrogen and feed the fuel gas to the gas turbine. The feed pressure on the turbine is as mentioned in *3.4.2.1 Feeding hydrogen rich fuel to the turbine,* at about 26.3bar. This means that as long as the pressure drop is below 13.9bar in the CO_2 capture unit and the mixer diluting the fuel there are no problematic pressure assumptions. This equals a pressure loss of over 30% which is very unlikely. It is more possible that the pressure loss is below 13.9bar and the fuel has to be choked before the combustion chamber. The choking is adjusted to the pressure ratio in the Power Island.

In further calculations on total plant efficiency it is assumed a compression cost of CO_2 of 0.11kWh per kilogram. The scrubbing cost is assumed to be 0.08kWh per kilogram CO_2 removed.

What this equals in the total plant is dependent on the results of the power island presented in *4.4 Power Island*. The impact carbon dioxide capture has on the total plant efficiency is therefore discussed in *4.5 IGCC Power Plant*.

4.4   Power Island

4.4.1   Gas Turbine

The composition presented in table 3.19 in *3.4.2.1 Feeding hydrogen rich gas to the turbine* is fed to the SGT5-4000F gas turbine and a simulation is run. The main results will be presented here. As mentioned in *3.4.2 Gas Turbine* there is done iterations to get a suitable amount of fuel.

4.4.1.1   Feeding hydrogen rich fuel to the turbine

There is also done a conversion to mass fraction for the fuel since GTPRO is operating with both molar and mass based flow. The mass fractions are used o find the absolute values of fuel needed.

Table 4.22. Molar and mass fraction fuel.

	Mol fraction fuel	Mass fraction fuel
Composition		
CO	0.021	0.039
CO_2	0.014	0.039
H_2	0.504	0.067
H_2O	0.000	0.000
N_2	0.461	0.855

With the SGT5-4000F turbine and the molar composition shown in table 4.22 the power output from the gas turbine becomes as shown in table 4.23.

Table 4.23. Power output.

Generated power		
Gas turbine	kW	262489
Steam turbine	kW	94950
Plant total	kW	357438

The steam cycle will be discussed later. There are possibilities for improvements when more steam is added from other processes in the plant. The gas turbine needs 75.69kg/s fuel to

produce this amount of power. This is a considerable higher amount than an equal turbine fired with natural gas. The same turbine fired with pure methane has a methane consumption of 11.69kg/s. The power output from the gas turbine is however reduced to 212MW because of the lower mass flow. Methane has a higher specific heating value than the diluted H_2 fuel. Methane has a LHV of 50047kJ/kg and the composition used here has a value of 8453kJ/kg. That justifies why the fuel amount using this composition is over 6 times higher than for pure methane. The chemical power input to the gas turbine can be calculated from the mass flow and the LHV for the fuel.

$$75.69\frac{kg}{s}\cdot 8453\frac{kJ}{kg} = 639808\frac{kJ}{s}$$

From this the efficiency for the power island can be calculated. This is so far not that interesting. Improvements on the steam cycle will increase the power output. In addition is this an IGCC plant where the chemical energy input to the whole plant is the coal. The coal goes through energy demanding processes before the power island. All of this has to be including when calculating overall efficiency. This will be discussed in *4.5 IGCC Power Plant*.

4.4.1.2　　Nitrogen, hydrogen and oxygen demand

The chosen gas turbine with the composition given in table 4.22 needs as mentioned a total fuel amount of 75.69kg/s. By using the total mass flow, the mass fractions and the molar weight for the substances one could find the demand of N_2, H_2 and O_2 at molar basis. This is necessary to get the values to fit into the PRO/II simulations. The PRO/II models that is run so far, calculates with an amount of 1kmol coal. Finding the absolute values of required H_2 will give the right amount of coal and then again the right amount of oxygen and steam. The nitrogen demand for this case is given in equation 4.24.

$$\dot{n}_{N_2} = 0.855\cdot 75.69\left[\frac{kg}{s}\right]\cdot \frac{1}{28.010\left[\frac{kg}{kmol}\right]} = 2.310\left[\frac{kmol}{s}\right] \qquad (4.24)$$

Similar for the hydrogen.

$$\dot{n}_{H_2} = 0.067 \cdot 75.690 \left[\frac{kg}{s} \right] \cdot \frac{1}{2.016 \left[\frac{kg}{kmol} \right]} = 2.519 \left[\frac{kmol}{s} \right] \tag{4.25}$$

The amount of H_2 calculated her is used to find the right amount of oxygen needed to get this level of H_2 from the Bituminous coal. As shown in the *4.2 Gasification Island,* 1kmol of coal gave 1.031kmol of H_2 reacting with 0.28kmol O_2. The ratio is then given in 4.26.

$$\frac{2.519}{1.031} = 2.442 \tag{4.26}$$

This indicates that there is a need 2.442kmol of the chosen coal and 2.442*0.28=0.684 kmol/s of O_2.

From the ASU part there has been found that the 1kmol of air is giving 0.216kmol of O_2 and 0.774kmol of N_2. Production of 0.684kmol of oxygen will then give 0.684*0.774/0.216=2.450kmol/s of N_2. This is a few percent more than the required amount of 2.310kmol/s. Because of this extra N_2 is available from the ASU. There are run simulations with more N_2 in the fuel. This results in a lower turbine inlet temperature and a lower power output. There is therefore decided to not increase the nitrogen amount even more.

4.4.1.3   Other results from the gas turbine calculations

Other results from the GTPRO simulations are shown in table 4.24.

Table 4.24. Other results from the gas turbine.

Stream	Pressure	Temperature	Mass flow
	bar	K	kg/s
Ambient air in	1.000	298.000	582.830
After filter	0.990	298.000	582.830
Compressor inlet	0.990	298.000	582.830
Turbine coolant			84.210
Compressor discharge	17.500	717.000	498.610
Fuel flow	26.260	380.000	75.690
Turbine inlet	16.970	1533.000	574.400
Turbine coolant			84.210
Turbine exhaust	1.030	814.000	658.520

The results from table 4.24 show that the turbine inlet temperature is lower than the expected values from table 3.17 in *3.4.2 Gas turbine*. A too low TIT reduces the power output and the efficiency in a gas turbine [16]. A low TIT increases the lifetime of a turbine [20]. There will be an evaluation what to prefer, a higher power production and efficiency or a longer lifetime. The reason for the relatively low TIT is probably the high concentration of nitrogen. A low temperature also lowers the NO_X formation. There is run a simulation where the H_2 amount is increased and the N_2 amount is decreased. This results in a higher TIT and a higher power output. But again it requires more H_2 and than again more O_2 to produce the H_2. This will give more N_2 production from the ASU. That will give a surplus of nitrogen since the demand in the gas turbine is decreased and the supply from the ASU is increased. The chosen fuel is kept. Improvements on efficiency will rather be done in the steam turbine process.

4.4.2   HRSG and Steam Turbine

Steam is both taken from the steam turbine, and fed into it at different temperatures and pressures. There are done calculations in the power cycle model in GTPRO and in the gasification model in PRO/II. These are adjusted so the steam consumption/production from each process can be integrated. The main results from these simulations will be presented here.

4.4.2.1 Utilizing steam from the steam turbine

The amount of steam utilized in the gasification process is determined from the wanted amount of fuel production required in the mentioned gas turbine process. From table 4.14 in *4.2.3.2 Gasification of Bituminous* and from table 4.21 in *4.2.5.1 Water gas shift reactor,* the steam demand for the gasification island for 1kmol coal is totally1.2kmol/s. 0.13kmol/s is utilized in the gasifier and 1.097kmol is used in the water gas shift reactors. To get the absolute value this is multiplied with the factor calculated in 4.26. That give a steam demand of 2.442*1.2kmol = 2.930kmol/s. The converting to kilogram per second is given in 4.26.

$$2.930 \left[\frac{kmol}{s} \right] \cdot 18.02 \left[\frac{kg}{kmol} \right] = 52.80 \left[\frac{kg}{s} \right] \tag{4.26}$$

This amount is taken from the turbine at 42.1bar and 529K. The gasification process modeled in PRO/II requires a pressure of 42bar and a temperature of 255˚C (528K). This will reduce the power output from the steam cycle. In the upcoming part, steam produced from heat in the gasification island, will be added to the turbine. This will gain the power output.

4.4.2.2 Adding steam to the steam turbine

There is decided to add steam at two pressure levels. This is suggested in GTPRO. There is suggested to add the steam at 34.47bar and at 3.447bar. The last pressure level is chosen for the low pressure part. The pressure level for the other stage is increased to 50bar. This is because the heat available in the gasification process can give steam at higher temperature than 529K which is the extracting point for steam at 42bar.

Production of steam at 50bar

This amount of steam is generated by two heat sources. The exhaust gas after the HRSG in the power island has a temperature of 463K, a mass flow of 658.52kg/s and a molar weight of 27.492kg/kmol. This is utilized to preheat the compressed water. The heat exchanger has a hot inlet - cold outlet approach of 5˚C which indicates that the water can reach a temperature of 458K or 185˚C. The syngas with temperature at about 1571˚C is utilized to generate steam and superheat it. The heat exchanger is set to give a steam outlet temperature of 344˚C. With that specification the amount of water is regulated until the syngas temperature reaches the wanted level of 250˚C. The results is collected in table 4.25.

Table 4.25. Temperatures in heat exchanging producing steam at 50bar.

		Stream		
		Exhaust gas	Syngas	Water
Mass flow	kg/s	658.520	53.139	50.979
Molar flow	kmol/s	23.953	2.678	2.829
Pressure	bar	1.030	41.600	50.000
T1	C	190.000		30.113
T2	C	144.114		185.000
T1	C		1570.583	185.000
T2	C		250.000	344.000

The syngas reached 250°C at a water amount of 2.829kmol/s. This is transformed to mass flow and implemented in the steam turbine model in GTPRO as 50.9kg/s at 50bar.

Production of steam at 3.447 bar

The gas between the two stages in the shift reactor is cooled before the second step to increase H_2 and CO_2 production. The cooling water used here is also integrated in the steam cycle. The same is the case for the heat exchanging after the whole gasification island where the water is condensed out. From GTPRO the required temperature at 3.447bar is 422K or 149°C. Both the heat exchangers are set to give a steam temperature of 149°C. In addition is the second heat exchanger also a splitter where the condensed water is removed from the stream before the acid gas remover. The water flow is regulated for both the heat exchangers until the conditions for each gas is as wanted. For the intermediate gas this is 225°C and for the H_2-rich gas this is condensing of in practical all the H_2O. The main results can be read from table 4.26.

Table 4.26. Temperatures in heat exchanging producing steam at 3.447 bar.

		Streams			
		Intermediate gas	Water	H_2-rich gas	Water
Mass flow	kg/s	100.211	20.146	100.211	34.058
Molar flow	kmol/s	5.291	1.118	5.291	1.890
Pressure	bar	41.000	3.447	40.600	3.447
T1	C	498.576	30.062	294.134	30.062
T2	C	225.000	149.000	36.673	149.000

From the table one can see that the total amount of low pressure steam becomes 20.146+34.058 ≈ 54.2kg/s. This was fed into the steam turbine.

4.4.3　　　*Overall view of the Power Island*

With a fuel composition as shown in table 4.22 in 4.4.1.1 and steam integrations as mentioned over, a power island simulation is run. The main data from this calculation will be shown here. A summary report including more details is listed in Appendix M**.**

Table 4.27. Final power output.

Generated power		
Gas turbine	kW	262489
Steam turbine	kW	124983
Plant total	kW	387472

Table 4.26 shows the power output from the combined cycle. The steam integration gives a higher power output from the steam cycle. Even though a considerable amount of steam is taken to the gasification process, the net power profit is positive.　The net power output from the gas turbine is the power remaining after all losses in the process. The main loss in a gas turbine process is the compressor work. From the GTPRO report the compressor work for this case is 252418kW. That includes compression of both air and fuel. In an IGCC plant is however some of the fuel already compressed before the power cycle. The nitrogen has to be compressed while the H_2-rich gas comes from the gasifier with a high pressure and is actually choked before the combustion chamber. In the GTPRO calculation the fuel compressing is found to be 18074kW. From table 4.22 it is shown that the volumetric N_2 part is about 50% of the total fuel. This implies that only about 9000kW is required to compress the N_2 part of the fuel. The H_2-rich gas is already is compressed in the gasification island. There is accordingly about 9000kW less loss than calculated.

On the other hand does the calculation not include the pumping work for the extra steam added at 50bar and at 3.447bar. A PRO/II simulation on this gives a total pumping work for these two pressure levels of about 300 kW, ergo there are still some "extra energy available".

An IGCC plant is a complex plant with a lot energy demanding processes that are not included in these simulations. There is therefore assumed that the 8500 kW will be utilized in other processes. The overall efficiency calculation will therefore not include this case.

The efficiency for the given combined cycle plant is then given in equation 4.27.

$$\eta_{cc} = \frac{P_{out}}{LHV_{in}} = \frac{387472}{639808} = 0.6056 \Rightarrow 60.56\% \tag{4.27}$$

Handling with an IGCC plant the overall efficiency will include losses in the ASU, in the gasification process etc. These will be discussed in the next chapter.

4.5 IGCC Power Plant

4.5.1 Initial calculation

The main numbers of the different islands is collected and set together in an Excel sheet. The feed to the gasifier is adjusted from the feed needed to the turbine in GTPRO. The feed to the ASU is again adjusted from the need in the gasifier. 96% of the CO_2 is removed after the shift reactor.

With the numbers given in the previous sections of *4 Results and Discussion* the following Excel sheet gives the overall plant calculations.

Table 4.28. Total IGCC power plant calculations.

Power Island		
Power output (GT+ST-C)	387472 kW	GTPRO simulation with SGT5-4000F
Gasification Island		
Coal feed to gasifier	2.442 kmol/s	Need of coal in gasifier to fit GTPRO
Coal molar weight	10.4545 kg/kmol	From element weight
Coal LHV (molar basis)	344372 kJ/kmol	Ultimate analysis of the coal
Coal LHV (mass basis)	32940 kJ/kg	Calculation based on the given numbers
Oxygen feed to gasifier	0.684 kmol/s	Need of oxygen in gasifer (from PRO/II)
Feed cost of coal	110 kW/kg	Approximate cost [6]
Escalated feed cost of coal	2808 kW	Adjusted the need of coal in gasifier
Air Separation Island		
Oxygen produced to gasifier	0.684 kmol/s	Incerted above
Oxygen production	0.216 kmol/s	per kmol/s of air (from PRO/II)
Nitrogen production	0.774 kmol/s	per kmol/s of air (from PRO/II)
Air compressor work	5673 kW	Oxygen delivered at 1.4 (from PRO/II)
After compression of oxygen	2598 kW	From 1.4 bar to 42 bar (from PRO/II)
Total compressor work	8271 kW	Air compression plus O_2 compression
Nitrogen prod., adjustes O_2 prod.	2.451 kmol/s	Fed to fuel before combustion
Escalated compressor work	26192 kW	Adjusted the need of O_2 in gasifier
Acid Gas Removal		
CO_2 captured (96% capture ratio)	0.664 kmol/s	per kmol/s coal
Molar weight CO_2	44.01 kg/kmol	Tabulated
CO_2 capture rate	29.22 kg/s	per kmol/s coal
CO_2 capture rate	105202 kg/h	per kmol/s coal
Compression cost	0.11 kWh/kg CO_2	From 1 to 110 bar [21]
Total compression cost	11572 kW	per kmol/s coal
Scrubbing cost	0.08 kWh/kg CO_2	[21]
Total scrubbing cost	8416 kW	per kmol/s coal
Escalated total CO_2 capture cost	48811 kW	Adjusted the coal fed to Gasification Isl.
CO_2 compression efficiency penalty	3.4 %	Calculation based on the given numbers
CO_2 scrubbing efficiency penalty	2.4 %	Calculation based on the given numbers
Total penalty by CO_2 capture	5.8 %	Calculation based on the given numbers
Total IGCC		
Power production without CO_2 cap.	358472 kW	Shift reactor included
Efficiency without CO_2 capture	42.6 %	Shift reactor included
Power production with CO_2 capture	309661 kW	
Efficiency with CO_2 capture	***36.8 %***	

Table 4.27 gives all the main numbers from the different islands in the IGCC power plant.

The numbers from the power island, air separation island, gasification island and acid gas

removal is discussed and presented in the previous sections of *4 Results and discussion* and will not be discussed particularly in this part of the report.

The most important numbers presented here are the efficiencies of the modeled plant. The overall efficiency without CO_2 capture is 42.6%. This number is although not particularly interesting due to the implemented shift reactor. An IGCC plant without CO_2 capture would not have a shift reactor included in the gasification island like this model has. The H_2 and CO rich syngas would be used directly as fuel gas and the efficiency would be higher.

The efficiency when carbon dioxide capture is included is very interesting. This number includes the losses by production and compression of oxygen and nitrogen, the coal feed cost, the production of high pressure steam to the gasifier and shift reactor, the removal and compression of CO_2 and pressure losses through the plant. An efficiency included CO_2 capture of 36.8% is a very satisfying result.

There are probably other losses not considered in this model. A real life power plant is also much more complex and advanced than a computer model. Complexity and units not considered in this model will probably reduce the efficiency. From *4.2.3.4 Comparison* the amount of produced syngas is calculated to be a bit higher than expected from literature. This will contribute to a higher overall efficiency. A lower production rate will decrease the efficiency. The efficiency of 36.8 percent is although very good and even with a reduction of 2-3 percentage points, the efficiency would still be satisfying.

4.5.2   Deviation from initial calculation

The numbers and efficiencies collected from the different islands are based on some initial assumptions. If these assumptions are changed it could have favourable impact on the total efficiency.

As mentioned *in 4.1.1.6 Overall GOX considerations* the polytrophic compressor efficiency in the air separation unit is sometimes assumed to be 90% instead of 85%. If the total IGCC plant calculations are performed with this assumption the efficiency with CO_2 capture is increased to 37.0%. An increase of 0.2 percentage points is not remarkable, but investing in

modern compressors with higher polytrophic efficiency is definitely a decision worth to consider.

The scrubbing and compression cost of CO2 is also very uncertain. As mentioned in *3.3.2 CO_2 capture unit* these costs are varying from 0.06-0.11 kWh per kilogram CO_2 removed in scrubbing cost and 0.11-0.13 kWh per kilogram CO_2 removed in compression cost. *In 4.3 Acid Gas Removal* it was decided to use an energy consumption of 0.08kWh for the scrubbing part and 0.11kWh for the compression part. A change in these numbers would also have major impacts on the total efficiency of the IGCC model.
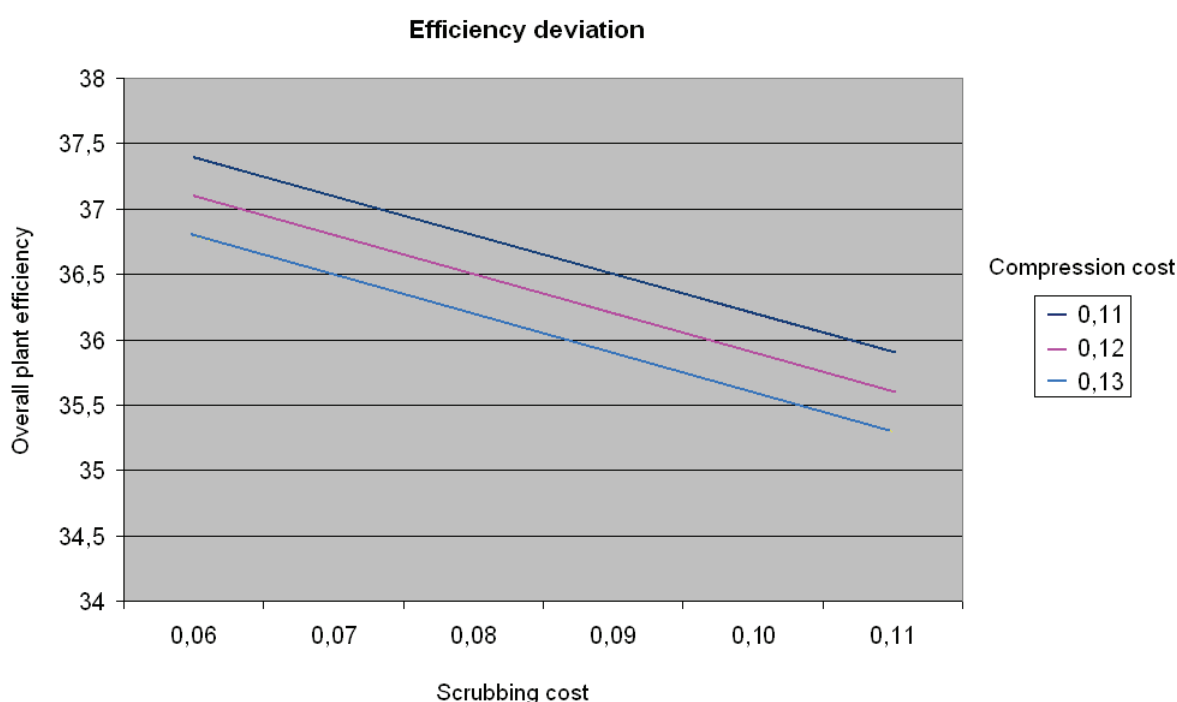
Figure 4.6. Efficiency deviation by changed CO_2 capture cost.

Figure 4.6 shows the deviation in efficiency for different CO_2 capture cost assumptions. The polytrophic compressor efficiency in the ASU is at the initial 85%.

The overall plant efficiency is very dependent of the carbon dioxide capture cost. The efficiency varies from 35.3% to 37.4% dependent on the capture costs assumed and wrong assumptions may therefore lead to remarkable efficiency surprises. Modern and well functional CO_2 scrubbers and compressors are therefore important to get the efficiency in a plant at a satisfying level.

4.5.3 Main numbers in favourable units

Through the report the production rates of the islands have mainly been describes in kmol/s. For simulations and integration between computer tools this is a favourable measure unit. The production rates of plants are although often referred in more understandable units as normal cubic meters per second (Nm^3) or tons per day (tons/day).

The numbers presented in this section is fitted the GTPRO simulation of 387472kW which equals about 387MW. This is only the GTPRO simulation and integrated with the other islands the output of the total plant is at about 310MW.

To produce the mentioned amount of electricity the Gasification Island must produce 59.6 Nm^3/s of H_2 rich gas. Per day this equals about 5.15 million Nm^3.

The production demand in the Gasification Island to fit the GTPRO simulation requires 2.442kmol/s of the given coal type. This equals about 2206tons/day.

To gasify this amount of coal it is needed 0.684kmol/s of oxygen produced in the Air Separation Island. 0.684kmol/s corresponds to 16.2 Nm^3/s or 1891tons/day.

5 Conclusion

Coal is the most common source for electricity production globally. The demand of power is increasing and new coal fired power plants are built continuous. IGCC is a technology giving incentives to CO_2 capture from coal fired power plants.

Integrated Gasification Combined Cycle consists of four main processes set together in a total IGCC power plant. The air separator produces oxygen which is fed to the gasification island together with steam and coal. In the gasifier coal is transformed to syngas consisting of mainly hydrogen and carbon monoxide. To be able to capture CO_2, the CO is reacted with steam in a shift reactor producing H_2 and CO_2. Carbon dioxide is removed by physical absorption before the H_2 rich fuel gas is diluted with nitrogen from the ASU and sent to the combustion chamber.

The air separation unit was modeled in PRO/II which is an excellent tool for cryogenic distillation. Under the given assumptions the ASU produces oxygen at an energy cost of 0.238kWh per kilogram pure oxygen delivered at 25°C and 1.4bar. The waste nitrogen is mainly utilized as diluter in the fuel gas. The products have a purity level at 95.6% for the oxygen and 99.6% for the nitrogen. Compared to industry standard both the energy consumption and product qualities are at satisfying levels.

The gasification island was also modeled in PRO/II. The program is not designed for solid fuels, but was verified as a proper tool for molar balance calculations. Comparison between PRO/II and results from an equilibrium calculator programmed in MatLab in addition to empirical data from a commercial entrained flow gasifier gave similar syngas compositions. The gasifier modeled has a Cold Gas Efficiency of 84.0% which is above the demand of a minimum of 78% to consider gasification feasible.

The acid gas removal is not modeled. A physical absorption process with selexol as solvent is reported to have a scrubber energy cost of 0.06-0.11kWh per kilogram CO_2 captured. In addition a compression cost of 0.11-0.13kWh per kilogram CO_2 must be included in the calculation. It is assumed a scrubber cost of 0.08 and a compression cost of 0.11kWh per kg CO_2 removed. Deviation in the assumed capture costs may change the calculated overall plant

efficiency with 1-2 percentage points. The CO_2 scrubber has a capture ratio of 96% and do also remove H_2S and other unwanted minor substances.

The power island is modeled in GTPRO which is a good tool for almost every power calculations. GTPRO is also able to model the gasification island, but this is as mentioned done in PRO/II. CO_2 and H_2S are removed from the fuel gas and nitrogen is added in an Excel sheet. In GTPRO a turbine able to handle large amounts of H_2 is chosen. The HRSG is integrated with the syngas cooler and produces steam to the gasification island in PRO/II.

Data from the four main processes are collected in an Excel sheet calculating the total efficiency of the plant. The overall efficiency of the IGCC power plant model ended at 36.8%. This number includes the losses by production and compression of oxygen and nitrogen, the coal feed cost, the production of high pressure steam to the gasifier and shift reactor, the removal and compression of CO_2 and pressure losses through the plant. The result is very satisfying compared to reports based on similar models.

In other models and in real life there might be units and losses not considered in this model. Changes in the assumptions may give great changes in the efficiency and should always be very well discussed.

6   Reference List

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Appendix Index

Appendix A   Chemical equilibrium derivation

Equilibrium equations

$$aA + bB \rightleftarrows cC + dD \tag{A1}$$

A, B, C and D are the substances and a, b, c and d are the molar amount of the substance.

For given temperatures an equilibrium constant K is tabulated for different equilibrium equations. The connection between the equilibrium constant and the molar fraction of the different substances in the equation are as follows [19].

$$K = \frac{(y_C^c)(y_D^d)}{(y_A^a)(y_B^b)} \left(\frac{p}{p_{ref}} \right)^{c+d-a-b} \tag{A2}$$

A detailed derivation of the equilibrium equation for CO is shown.

$$C + 1/2 O_2 \rightleftarrows CO \tag{2.30}$$

Inserted in equation A2.

$$K_{CO} = \frac{[y_{CO}]^1}{[y_C]^1 [y_{O_2}]^{\frac{1}{2}}} \left(\frac{p}{p_{ref}} \right)^{1-1-1/2} = \frac{[y_{CO}]}{[y_C][y_{O_2}]^{\frac{1}{2}}} \left(\frac{p}{p_{ref}} \right)^{-1/2} \tag{A3}$$

Assuming $p_{ref} = 1$ gives

$$K_{CO} = \frac{[y_{CO}]}{[y_C][y_{O_2}]^{\frac{1}{2}} p^{\frac{1}{2}}} \tag{2.40}$$

Corresponding derivation are done for the other six formation reactions.

$$C + O_2 \rightarrow CO_2 \quad (2.31) \qquad \Rightarrow \qquad K_{CO_2} = \frac{[y_{CO_2}]}{[y_C][y_{O_2}] p} \quad (2.41)$$

$$C + 2H_2 \rightleftarrows CH_4 \quad (2.33) \qquad \Rightarrow \qquad K_{CH_4} = \frac{[y_{CH_4}]}{[y_C][y_{H_2}]^2 p^2} \quad (2.43)$$
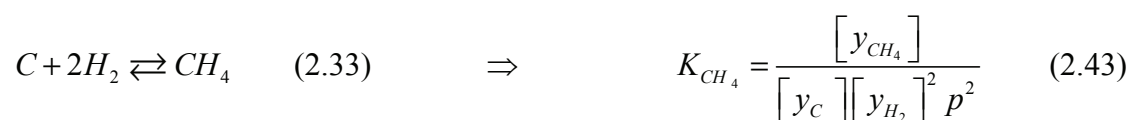
$$H_2 + 1/2\,O_2 \rightleftarrows H_2O \quad (2.35) \qquad \Rightarrow \qquad K_{H_2O} = \frac{\left[y_{H_2O} \right]}{\left[y_{H_2} \right]\left[y_{O_2} \right] p^{\frac{1}{2}}} \qquad (2.42)$$

$$1/2\,N_2 + 1/2\,O_2 \rightleftarrows NO \quad (2.36) \qquad \Rightarrow \qquad K_{NO} = \frac{\left[y_{NO} \right]}{\left[y_{O_2} \right]^{\frac{1}{2}}\left[y_{N_2} \right]^{\frac{1}{2}}} \qquad (2.44)$$

$$S + O_2 \rightleftarrows SO_2 \qquad (2.37) \qquad \Rightarrow \qquad K_{SO_2} = \frac{\left[y_{SO_2} \right]}{\left[y_S \right]\left[y_{O_2} \right] p} \qquad (2.45)$$

$$S + H_2 \rightleftarrows H_2S \qquad (2.38) \qquad \Rightarrow \qquad K_{H_2S} = \frac{\left[y_{H_2S} \right]}{\left[y_S \right]\left[y_{H_2} \right] p} \qquad (2.46)$$

Appendix B   MatLab fsolve function

```matlab
function F=syngascomp(X)

%Only insert numbers between the dotted lines
%---------------------------------------------------------------------------
p       = 42;        %Insert gasifier pressure
T       = 1846;      %Insert gasifier temperature in Kelvin
Cf      = 0.596;     %Insert amount of C in coal in mole fraction
Hf      = 0.346;     %Insert amount of H in coal in mole fraction
Of      = 0.050;     %Insert amount of O in coal in mole fraction
H2Of    = 0.13;      %Insert feed of H2O to gasifier in moles
O2f     = 0.28;      %Insert feed of O2 to gasifier in moles
%---------------------------------------------------------------------------
%Do not insert any numbers below this line

%Defining the mole fractions as X's
yCO     = X(1);
yCO2    = X(2);
yH2     = X(3);
yH2O    = X(4);
n       = X(5);

%Tabulated K-values for: CO2 + H2 <=> CO +H2O
K298    =-5.018;
K500    =-2.139;
K1000   =-0.159;
K1200   = 0.135;
K1400   = 0.333;
K1600   = 0.474;
K1700   = 0.530;
K1800   = 0.577;
K1900   = 0.619;
K2000   = 0.656;
K2100   = 0.688;
K2200   = 0.716;

%Interpolating K-value for any given temperature between 298 and 2200K
t = 298;
if t<T
    while t<T
    t=t+1;
    end
    if t<298
        disp('The temperature is out of range')
        K   = 1;
    elseif t<500
        K   = 10^(((t-298)/(500-298))*(K500-K298)+K298);
    elseif t<1000
        K   = 10^(((t-500)/(1000-500))*(K1000-K500)+K500);
    elseif t<1200
        K   = 10^(((t-1000)/(1200-1000))*(K1200-K1000)+K1000);
    elseif t<1400
        K   = 10^(((t-1200)/(1400-1200))*(K1400-K1200)+K1200);
    elseif t<1600
        K   = 10^(((t-1400)/(1600-1400))*(K1600-K1400)+K1400);
    elseif t<1700
        K   = 10^(((t-1600)/(1700-1600))*(K1700-K1600)+K1600);
    elseif t<1800
        K   = 10^(((t-1700)/(1800-1700))*(K1800-K1700)+K1700);
    elseif t<1900
        K   = 10^(((t-1800)/(1900-1800))*(K1900-K1800)+K1800);
    elseif t<2000
        K   = 10^(((t-1900)/(2000-1900))*(K2000-K1900)+K1900);
    elseif t<2100
        K   = 10^(((t-2000)/(2100-2000))*(K2100-K2000)+K2000);
```

```
    elseif t<2200
        K   = 10^(((t-2100)/(2200-2100))*(K2200-K2100)+K2100);
    else
        disp('The temperature is out of range')
        K   = 1;
    end
else
end

Kuse    =1/K; %The tabulated K-values are for reaction going
              %the other way and K must be set to 1/K

%Calculation of element feeds
nCfeed  = Cf;                    %Total feed of C
nOfeed  = Of + H2Of + 2*O2f;     %Total feed of O
nHfeed  = Hf + 2*H2Of;           %Total feed of H

%The five equations
F(1)    = (2*yH2 + 2*yH2O)*n - nHfeed;        %H2 element mass balance
F(2)    = (yCO + 2*yCO2 + yH2O)*n - nOfeed;   %O2 element mass balance
F(3)    = (yCO + yCO2)*n - nCfeed;            %C element mass balance
F(4)    = yCO + yCO2 + yH2O + yH2 - 1;        %Total mass balance
F(5)    = (((yCO2)*(yH2))/((yH2O)*(yCO)))-Kuse; %Equilibrium equation

%Displaying the iterated answers
disp(['yCO  = ' num2str(yCO)]);
disp(['yCO2 = ' num2str(yCO2)]);
disp(['yH2  = ' num2str(yH2)]);
disp(['yH2O = ' num2str(yH2O)]);
disp(['n    = ' num2str(n)]);
disp(' ');
```

Appendix C   MatLab run fsolve function

```
%Programname: calculatesyngas
%The script runs the fsolve function for syngascomp

%Start values for the composition
yCO      = 0.5;
yCO2     = 0.5;
yH2      = 0.5;
yH2O     = 0.5;
n        = 1.2;

fsolve('syngascomp',[yCO yCO2 yH2 yH2O n]);
```

Appendix D   Coal as gas compared with chosen coal composition

Table D1 shows the coal composition containing fixed carbon and the gaseous substitute.

Table D1. Coal composition of coal containing fixed carbon and a gaseous substitute

Composition	Coal	Coal as gaseous substances
C	0.700	0.000
H_2	0.100	0.000
O_2	0.100	0.000
N_2	0.050	0.050
S	0.050	0.050
CO	0.000	0.550
CO_2	0.000	0.100
CH_4	0.000	0.050

The gaseous substitute for coal contains 0.275 more moles of O_2 than the fixed carbon composition. This inequality must be compensated for by subtract 0.275 moles on the oxygen consumption for the gaseous substitute when the compositions are compared.

The model with carbon as a solid was arranged to with a 98% CO shift as a condition for the gasifier. The same CO shift rate was implemented in the coal as gas model to compare the compositions in the syngas. The results are presented in table D2.

Table D2. Gaseous substitute with optimized O_2 and H_2O amounts.

	Coal	Oxygen	Water to gasifier	Syngas	Water to shift	H_2 rich gas
Temperature	15.000	15.000	300.000	1787.728	180.000	20.000
Pressure	8.000	8.000	8.000	7.900	7.900	7.900
Flowrate	0.800	0.007	0.178	1.105	0.591	1.696
Composition						
C	0.000	0.000	0.000	0.000	0.000	0.000
CO	0.688	0.000	0.000	0.627	0.000	0.012
CO_2	0.125	0.000	0.000	0.006	0.000	0.401
O_2	0.000	1.000	0.000	0.024	0.000	0.016
H_2	0.000	0.000	0.000	0.177	0.000	0.512
H_2O	0.000	0.000	1.000	0.075	1.000	0.000
CH_4	0.063	0.000	0.000	0.000	0.000	0.000
N_2	0.063	0.000	0.000	0.045	0.000	0.029
NO	0.000	0.000	0.000	0.000	0.000	0.000
S	0.063	0.000	0.000	0.000	0.000	0.000
SO_2	0.000	0.000	0.000	0.045	0.000	0.029
H_2S	0.000	0.000	0.000	0.000	0.000	0.000

Because of the surplus of 0.275 moles of oxygen in the gaseous coal substitute compared with the fixed carbon coal composition the comparable oxygen flowrate for the substitute should be 0.007 + 0.275 = 0.282. The use of oxygen in the two simulations is then approximately equal.

The two simulations main data are compared in table D3. In table D3 the shaded areas are for the coal defined as a gaseous substitute while the white areas are for coal containing fixed carbon

Table D3. Comparison of fixed carbon and gaseous substitute.

	Coal	Coal	Syngas	Syngas	H$_2$ rich gas	H$_2$ rich gas
Composition						
C	0.700	0.000	0.000	0.000	0.000	0.000
CO	0.000	0.550	0.692	0.693	0.019	0.020
CO$_2$	0.000	0.100	0.008	0.007	0.680	0.680
O$_2$	0.100	0.000	0.047	0.027	0.047	0.027
H$_2$	0.100	0.000	0.231	0.196	0.902	0.868
H$_2$O	0.000	0.000	0.124	0.083	0.000	0.000
CH$_4$	0.000	0.050	0.000	0.000	0.000	0.000
N$_2$	0.050	0.050	0.050	0.050	0.051	0.049
NO	0.000	0.000	0.000	0.000	0.000	0.000
S	0.050	0.050	0.000	0.000	0.000	0.000
SO$_2$	0.000	0.000	0.050	0.050	0.051	0.049
H$_2$S	0.000	0.000	0.000	0.000	0.000	0.000

The gas composition, both for syngas and H$_2$ rich gas, is quite similar for coal defined as fixed carbon and defined as a gaseous mixture. But there are some differences due to different steam and oxygen consumption. It looks like fixed carbon is handled by PRO/II, but to be sure an extra simulation is run.

Appendix E   Stream properties for initial GOX

Table E1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6-1	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Mixed
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	100.796
Pressure	bar	1.000	1.570	2.450	3.920	6.300	6.300	6.100
Flowrate	kmol/s	0.990	0.990	0.990	0.990	0.990	0.213	0.213
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A6-2	A7-2	A8	A9-1	A9-2	A10-2
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	102.780	102.116	102.151	102.151	94.344
Pressure	bar	6.300	6.100	6.000	6.000	6.000	1.250
Flowrate	kmol/s	0.777	0.777	0.990	0.900	0.090	0.090
Composition							
O_2		0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009

Table E2. Stream properties of oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5	OX6	OX7	OX8	OX9
Phase		Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Vapor
Temperature	K	100.623	83.024	93.642	94.004	94.004	93.642	93.750	94.338	296.977
Pressure	bar	6.000	1.250	1.500	1.500	1.500	1.500	1.500	1.500	1.500
Flowrate	kmol/s	0.463	0.463	0.447	0.381	0.066	0.150	0.216	0.216	0.216
Composition										
O_2		0.403	0.403	0.950	0.946	0.971	0.950	0.956	0.956	0.956
N_2		0.584	0.584	0.014	0.015	0.004	0.014	0.011	0.011	0.011
AR		0.013	0.013	0.036	0.038	0.025	0.036	0.033	0.033	0.033

Table E3. Stream properties of nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6	NI7	NI8
Phase		Vapor	Mixed	Mixed	Mixed	Mixed	Vapor	Vapor	Vapor
Temperature	K	95.338	95.256	95.246	95.246	77.431	77.434	94.256	297.000
Pressure	bar	5.500	5.500	5.500	5.500	1.000	1.000	1.000	1.000
Flowrate	kmol/s	0.437	0.437	0.437	0.437	0.437	0.774	0.774	0.774
Composition									
O_2		0.005	0.005	0.005	0.005	0.005	0.002	0.002	0.002
N_2		0.990	0.990	0.990	0.990	0.990	0.996	0.996	0.996
AR		0.005	0.005	0.005	0.005	0.005	0.002	0.002	0.002

Appendix F   Stream and compressor properties for improved CCR

Table F1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6-1	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Liquid
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	94.108
Pressure	bar	1.000	1.520	2.350	3.670	5.800	5.800	5.600
Flowrate	kmol/s	0.990	0.990	0.990	0.990	0.990	0.213	0.213
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A6-2	A7-2	A8	A9-1	A9-2	A10-2
Phase		Vapor	Vapor	Mixed	Mixed	Mixed	Mixed
Temperature	K	298.000	101.028	98.770	98.770	98.770	82.961
Pressure	bar	5.800	5.600	5.500	5.500	5.500	1.250
Flowrate	kmol/s	0.777	0.777	0.990	0.900	0.090	0.090
Composition							
O_2		0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009

Table F2. Stream properties for oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5	OX6	OX7	OX8	OX9
Phase		Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Vapor
Temperature	K	98.772	82.415	93.484	93.964	93.964	93.484	93.624	93.108	297.000
Pressure	bar	5.500	1.250	1.500	1.500	1.500	1.500	1.500	1.500	1.500
Flowrate	kmol/s	0.535	0.535	0.344	0.281	0.063	0.150	0.213	0.213	0.213
Composition										
O_2		0.349	0.349	0.950	0.945	0.973	0.950	0.957	0.957	0.957
N_2		0.638	0.638	0.020	0.023	0.006	0.020	0.016	0.016	0.016
AR		0.012	0.012	0.030	0.032	0.021	0.030	0.027	0.027	0.027

Table F3. Stream properties for nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6	NI7	NI8
Phase		Vapor	Vapor	Mixed	Mixed	Mixed	Vapor	Vapor	Vapor
Temperature	K	94.126	94.624	94.087	94.027	77.431	77.532	93.624	297.000
Pressure	bar	5.000	5.000	5.000	5.000	1.000	1.000	1.000	1.000
Flowrate	kmol/s	0.365	0.365	0.365	0.365	0.365	0.777	0.777	0.777
Composition									
O_2		0.006	0.006	0.006	0.006	0.006	0.005	0.005	0.005
N_2		0.990	0.990	0.990	0.990	0.990	0.991	0.991	0.991
AR		0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004

Table F4 Unit properties for compressor work.

Compressor Name		C1	C2	C3	C4
Pressure	bar	1.550	2.400	3.750	5.930
Temperature	K	345.247	347.402	348.648	350.131
Head	M	4844.730	5065.519	5192.617	5343.484
Actual Work	kW	1362.509	1424.603	1460.347	1502.777
Isentropic coef., k		1.401	1.402	1.404	1.407

Total compressor work for 0.99kmol/s dry air is 5750kW.

Compression of moist in the air equals:

$$\frac{0.01 kmol_{H_2O}}{0.99 kmol_{Air}} \cdot 5750kW \cdot \frac{18.02 kg/kmol_{H_2O}}{28.96 kg/kmol_{Air}} = 36kW$$

Total compression of 1kmol/s moist air is then 5786kW.

Appendix G   Stream properties for modifications in the main heat exchanger

Table G1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6-1	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	100.859
Pressure	bar	1.000	1.570	2.450	3.920	6.300	6.300	6.100
Flowrate	kmol/s	0.990	0.990	0.990	0.990	0.990	0.213	0.213
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A6-2	A7-2	A6-3	A7-3	A8-3	A8
Phase		Vapor	Mixed	Vapor	Vapor	Vapor	Mixed
Temperature	K	298.000	100.776	298.000	210.000	131.556	100.565
Pressure	bar	6.300	6.100	6.300	6.300	1.250	6.000
Flowrate	kmol/s	0.697	0.697	0.080	0.080	0.080	0.910
Composition							
O_2		0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009

Table G2. Stream properties for oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5	OX6	OX7	OX8	OX9
Phase		Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Vapor
Temperature	K	100.568	82.976	93.644	94.005	94.005	93.644	93.752	94.339	297.000
Pressure	bar	6.000	1.250	1.500	1.500	1.500	1.500	1.500	1.500	1.500
Flowrate	kmol/s	0.473	0.473	0.444	0.378	0.065	0.150	0.215	0.215	0.215
Composition										
O_2		0.399	0.399	0.950	0.946	0.971	0.950	0.956	0.956	0.956
N_2		0.588	0.588	0.014	0.015	0.004	0.014	0.011	0.011	0.011
AR		0.013	0.013	0.036	0.038	0.025	0.036	0.033	0.033	0.033

Table G3. Stream properties for nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6
Phase		Vapor	Mixed	Mixed	Mixed	Mixed	Vapor
Temperature	K	95.339	95.257	95.246	95.246	77.431	77.434
Pressure	bar	5.500	5.500	5.500	5.500	1.000	1.000
Flowrate	kmol/s	0.437	0.437	0.437	0.437	0.437	0.774
Composition							
O_2		0.005	0.005	0.005	0.005	0.005	0.002
N_2		0.990	0.990	0.990	0.990	0.990	0.996
AR		0.005	0.005	0.005	0.005	0.005	0.002

Stream Name		NI7	NI8-1	NI9-1	NI8-2	NI9-2	NI10
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	94.257	94.257	296.657	94.257	203.214	288.803
Pressure	bar	1.000	1.000	1.000	1.000	1.000	1.000
Flowrate	kmol/s	0.774	0.709	0.709	0.065	0.065	0.774
Composition							
O_2		0.002	0.002	0.002	0.002	0.002	0.002
N_2		0.996	0.996	0.996	0.996	0.996	0.996
AR		0.002	0.002	0.002	0.002	0.002	0.002

Appendix H   Number of compressors in ASU model

Total work to compress 1 kmol/s of dry air for different number of compressors.

Table H1. One compressor.

Compressor Name		C1	Total work
Pressure	bar	6.430	
Temperature	K	552.722	
Head	M	26479.143	
Actual Work	kW	7522.091	7522.091
Isentropic coef.. k		1.398	

Table H2. Two compressors.

Compressor Name		C1	C2	Total work
Pressure	bar	2.500	6.430	
Temperature	K	405.062	411.718	
Head	M	11009.189	11699.027	
Actual Work	kW	3127.447	3323.414	6450.861
Isentropic coef.. k		1.401	1.404	

Table H3. Three compressors.

Compressor Name		C1	C2	C3	Total work
Pressure	bar	1.800	3.300	6.430	
Temperature	K	362.975	367.981	375.469	
Head	M	6667.510	7181.967	7952.191	
Actual Work	kW	1894.080	2040.225	2259.028	6193.333
Isentropic coef.. k		1.401	1.403	1.406	

Table H4. Four compressors.

Compressor Name		C1	C2	C3	C4	Total work
Pressure	bar	1.500	2.300	3.800	6.430	
Temperature	K	341.472	346.342	355.338	358.132	
Head	M	4457.062	4956.693	5880.362	6166.210	
Actual Work	kW	1266.145	1408.078	1670.470	1751.673	6096.366
Isentropic coef.. k		1.401	1.402	1.404	1.407	

Table H5. Five compressors.

Compressor Name		C1	C2	C3	C4	C5	Total work
Pressure	bar	1.400	2.000	2.900	4.200	6.430	
Temperature	K	333.661	338.384	339.919	339.874	345.545	
Head	M	3655.170	4139.551	4296.444	4290.852	4871.360	
Actual Work	kW	1038.346	1175.948	1220.517	1218.929	1383.837	6037.576
Isentropic coef.. k		1.401	1.402	1.403	1.405	1.407	

Table H6. Six compressors.

Compressor Name		C1	C2	C3	C4	C5	C6	Total work
Pressure	bar	1.300	1.700	2.300	3.200	4.500	6.430	
Temperature	K	325.465	327.814	332.508	334.944	335.964	338.278	
Head	M	2814.229	3054.921	3536.059	3785.374	3888.934	4125.394	
Actual Work	kW	799.455	867.830	1004.510	1075.334	1104.753	1171.926	6023.808

Table H7. Total work for different number of compressors.

Number of compressors	Total work [kW]
1	7522
2	6451
3	6193
4	6096
5	6038
6	6024

Figure 4.2 is made directly from table H7.

Calculation of energy consumption per kilogram of produced oxygen for different number of compressors.

One compressor:

$$\frac{7522kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.3162kW/kg_{O_2}$$

Two compressors:

$$\frac{6451kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.2712kW/kg_{O_2}$$

Three compressors:

$$\frac{6193kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.2603kW/kg_{O_2}$$

Four compressors:

$$\frac{6096kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.2563kW/kg_{O_2}$$

Five compressors:

$$\frac{6038kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.2538kW/kg_{O_2}$$

Six compressors:

$$\frac{6024kW}{0.216kmol/s \cdot 0.956kmol_{O_2}/kmol \cdot 32.00kg_{O_2}/kmol_{O_2} \cdot 3600s/h} = 0.2532kW/kg_{O_2}$$

It is possible to maximize the distribution of compressor work between the compressors in the different cases. These are therefore not necessarily the best solutions, but close enough to give directions in the decision making.

Appendix I   Stream properties for min number of trays

Table I1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6-1	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	104.539
Pressure	bar	1.000	1.570	2.450	3.920	6.300	6.300	6.100
Flowrate	kmol/s	0.990	0.990	0.990	0.990	0.990	0.213	0.213
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A6-2	A7-2	A8	A9-1	A9-2	A10-2
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	101.985	102.372	102.257	102.257	94.466
Pressure	bar	6.300	6.100	6.000	6.000	6.000	1.250
Flowrate	kmol/s	0.777	0.777	0.990	0.900	0.090	0.090
Composition							
O_2		0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009

Table I2. Stream properties for oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5	OX6	OX7	OX8	OX9
Phase		Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Vapor
Temperature	K	100.247	82.689	93.634	94.006	94.006	93.634	93.740	94.357	297.000
Pressure	bar	6.000	1.250	1.500	1.500	1.500	1.500	1.500	1.500	1.500
Flowrate	kmol/s	0.501	0.501	0.471	0.409	0.061	0.150	0.211	0.211	0.211
Composition										
O_2		0.371	0.371	0.950	0.947	0.971	0.950	0.956	0.956	0.956
N_2		0.615	0.615	0.014	0.016	0.004	0.014	0.011	0.011	0.011
AR		0.014	0.014	0.036	0.038	0.025	0.036	0.033	0.033	0.033

Table I3. Stream properties for nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6	NI7	NI8
Phase		Vapor	Mixed	Mixed	Mixed	Mixed	Vapor	Vapor	Vapor
Temperature	K	95.357	95.259	95.247	95.247	77.431	77.561	94.259	297.000
Pressure	bar	5.500	5.500	5.500	5.500	1.000	1.000	1.000	1.000
Flowrate	kmol/s	0.399	0.399	0.399	0.398	0.398	0.778	0.778	0.778
Composition									
O_2		0.008	0.008	0.008	0.008	0.008	0.007	0.007	0.007
N_2		0.990	0.990	0.990	0.990	0.990	0.990	0.990	0.990
AR		0.002	0.002	0.002	0.002	0.002	0.003	0.003	0.003

Appendix J   Properties of the optimal GOX model

Table J1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6-1	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Mixed
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	99.207
Pressure	bar	1.000	1.520	2.300	3.570	5.600	5.600	5.400
Flowrate	kmol/s	0.990	0.990	0.990	0.990	0.990	0.213	0.213
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A6-2	A7-2	A6-3	A7-3	A8-3	A8
Phase		Vapor	Mixed	Vapor	Vapor	Vapor	Mixed
Temperature	K	298.000	99.153	298.000	185.000	132.246	98.928
Pressure	bar	5.600	5.400	5.600	5.600	1.250	5.300
Flowrate	kmol/s	0.687	0.687	0.090	0.090	0.090	0.900
Composition							
O_2		0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009

Table J2. Stream properties for oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5	OX6	OX7	OX8	OX9
Phase		Liquid	Mixed	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Vapor
Temperature	K	98.915	82.979	92.924	93.295	93.295	92.924	93.035	93.374	296.974
Pressure	bar	5.300	1.250	1.400	1.400	1.400	1.400	1.400	1.400	1.400
Flowrate	kmol/s	0.462	0.462	0.434	0.368	0.066	0.150	0.216	0.216	0.216
Composition										
O_2		0.404	0.404	0.950	0.946	0.971	0.950	0.956	0.956	0.956
N_2		0.582	0.582	0.014	0.016	0.004	0.014	0.011	0.011	0.011
AR		0.014	0.014	0.036	0.038	0.025	0.036	0.033	0.033	0.033

Table J3. Stream properties for nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6
Phase		Vapor	Mixed	Mixed	Mixed	Mixed	Vapor
Temperature	K	94.374	94.289	94.279	94.279	78.242	78.249
Pressure	bar	5.100	5.100	5.100	5.100	1.100	1.100
Flowrate	kmol/s	0.438	0.438	0.438	0.438	0.438	0.774
Composition							
O_2		0.006	0.006	0.006	0.006	0.006	0.002
N_2		0.990	0.990	0.990	0.990	0.990	0.996
AR		0.004	0.004	0.004	0.004	0.004	0.002

Stream Name		NI7	NI8-1	NI9-1	NI8-2	NI9-2	NI10
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	93.289	93.289	294.752	93.289	250.943	291.074
Pressure	bar	1.100	1.100	1.100	1.100	1.100	1.100
Flowrate	kmol/s	0.774	0.709	0.709	0.065	0.065	0.774
Composition							
O_2		0.002	0.002	0.002	0.002	0.002	0.002
N_2		0.996	0.996	0.996	0.996	0.996	0.996
AR		0.002	0.002	0.002	0.002	0.002	0.002

Table J4. Compressor properties.

Compressor Name		C1	C2	C3	C4
Pressure	bar	1.550	2.350	3.650	5.730
Temperature	K	345.247	344.959	348.003	349.345
Head	M	4844.730	4814.545	5126.344	5262.898
Actual Work	kW	1362.509	1354.020	1441.709	1480.113
Isentropic coef.. k		1.401	1.402	1.404	1.406

Compression work for compression of 0.99kmol/s of dry air is 5638kW.

Additional work for compression of 0.01kmol/s of water vapor is

$$\frac{0.01 kmol_{H_2O}}{0.99 kmol_{Air}} \bullet 5638 kW \bullet \frac{18.02 kg / kmol_{H_2O}}{28.96 kg / kmol_{Air}} = 35 kW$$

Compression work of 1.00kmol/s of moist air is then 5673kW.

Table J5. Heat exchanger properties.

Hx Name		E1	E2	E3	E4	E5	E6
		Main heat ex	Main heat ex	Subcooler	Subcooler	Convergence	Comb cond-reb
Duty	MW	1.2812	4.1899	1.4702	0.3507	0.0007	2.5098

Table J6. Column properties.

Column Name		HP	LP
Condenser Duty	MW	-2.5098	n/a
Reboiler Duty	MW	n/a	-0.0003

Appendix K   Stream properties LOX

Table K1. Stream properties of air.

Stream Name		A1	A2	A3	A4	A5	A6	A7-1
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	298.000	298.000	298.000	298.000	298.000	298.000
Pressure	bar	1.000	1.570	2.450	3.920	6.300	6.300	6.300
Flowrate	kmol/s	0.990	0.990	1.190	1.190	1.190	0.890	0.445
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Stream Name		A7-2	A7-3	A8-1	A8-2	A8-3	A9	A10
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	298.000	101.450	101.050	101.738	101.241	100.585
Pressure	bar	6.300	6.300	6.100	6.100	6.100	6.000	6.000
Flowrate	kmol/s	0.245	0.200	0.445	0.245	0.200	0.890	0.890
Composition								
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009

Table K2. Stream properties of booster compressed air.

Stream Name		B1	B2	B3	B4	B5	B6-1	B6-2	B7-1	B7-2
Phase		Vapor	Vapor	Liquid	Mixed	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	298.000	298.000	106.000	83.336	94.305	94.305	94.305	297.000	93.764
Pressure	bar	6.300	40.000	39.000	1.570	1.570	1.570	1.570	1.570	1.250
Flowrate	kmol/s	0.300	0.300	0.300	0.300	0.300	0.200	0.100	0.200	0.100
Composition										
O_2		0.210	0.210	0.210	0.210	0.210	0.210	0.210	0.210	0.210
N_2		0.781	0.781	0.781	0.781	0.781	0.781	0.781	0.781	0.781
AR		0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009

Table K3. Stream properties for oxygen.

Stream Name		OX1	OX2	OX3	OX4	OX5
Phase		Liquid	Mixed	Liquid	Vapor	Liquid
Temperature	K	100.588	82.993	93.628	94.001	94.001
Pressure	bar	6.000	1.250	1.500	1.500	1.500
Flowrate	kmol/s	0.461	0.461	0.438	0.372	0.066
Composition						
O_2		0.400	0.400	0.950	0.946	0.971
N_2		0.587	0.587	0.014	0.016	0.004
AR		0.013	0.013	0.036	0.038	0.025

Stream Name		OX6	OX7	OX8	OX9	OX10
Phase		Liquid	Mixed	Liquid	Liquid	Vapor
Temperature	K	93.628	93.740	93.889	94.339	297.000
Pressure	bar	1.500	1.500	42.000	42.000	42.000
Flowrate	kmol/s	0.150	0.216	0.216	0.216	0.216
Composition						
O_2		0.950	0.956	0.956	0.956	0.956
N_2		0.014	0.011	0.011	0.011	0.011
AR		0.036	0.032	0.032	0.032	0.032

Table K4. Stream properties for nitrogen.

Stream Name		NI1	NI2	NI3	NI4	NI5	NI6
Phase		Vapor	Mixed	Mixed	Mixed	Mixed	Vapor
Temperature	K	95.339	95.338	95.305	95.246	77.432	77.437
Pressure	bar	5.500	5.500	5.500	5.500	1.000	1.000
Flowrate	kmol/s	0.429	0.429	0.429	0.429	0.429	0.774
Composition							
O_2		0.005	0.005	0.005	0.005	0.005	0.002
N_2		0.990	0.990	0.990	0.990	0.990	0.996
AR		0.005	0.005	0.005	0.005	0.005	0.002

Stream Name		NI7	NI8-1	NI8-2	NI9-1	NI9-2	NI10
Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Temperature	K	94.338	94.338	94.338	297.000	296.910	296.939
Pressure	bar	1.000	1.000	1.000	1.000	1.000	1.000
Flowrate	kmol/s	0.774	0.247	0.527	0.247	0.527	0.774
Composition							
O_2		0.002	0.002	0.002	0.002	0.002	0.002
N_2		0.996	0.996	0.996	0.996	0.996	0.996
AR		0.002	0.002	0.002	0.002	0.002	0.002

Appendix L Chemical Calculator example

Table L1 shows a transcript of one of the online equilibrium calculations. The other calculations followed the same principles. The online web address to the chemical calculator is given in the reference list at [26].

Table L1. Results from online chemical calculator.

Chemical Equilibrium Results

	Initial State	Equilibrium State
Pressure (atm)	5.1320E+01	5.1320E+01
Temperature (K)	1.1805E+03	1.8453E+03
Volume (cm^3/g)	1.3471E+02	1.3471E+02
Enthalpy (erg/g)	2.6207E+11	-2.7702E+10
Internal Energy (erg/g)	2.5507E+11	-3.4707E+10
Entropy (erg/g K)	1.2299E+08	9.9956E+07

	Initial State		Equilibrium State	
	mole fraction	mass fraction	mole fraction	mass fraction
C	4.2300E-01	3.6259E-01	2.7072E-16	1.4847E-16
H	2.4556E-01	1.7665E-02	3.5000E-05	1.6108E-06
O	3.5486E-02	4.0519E-02	1.1859E-10	8.6633E-11
N	3.5486E-03	3.5472E-03	5.8572E-13	3.7459E-13
S	1.4194E-03	3.2481E-03	2.0406E-07	2.9875E-07
H_2O	9.2264E-02	1.1862E-01	9.7516E-02	8.0214E-02
O_2	1.9872E-01	4.5381E-01	2.1573E-11	3.1519E-11
CO	0.0000E+00	0.0000E+00	5.9886E-01	7.6591E-01
CO_2	0.0000E+00	0.0000E+00	6.2254E-02	1.2510E-01
H_2	0.0000E+00	0.0000E+00	2.3631E-01	2.1751E-02
NO	0.0000E+00	0.0000E+00	3.0979E-09	4.2443E-09
SO_2	0.0000E+00	0.0000E+00	5.7825E-07	1.6914E-06
H_2S	0.0000E+00	0.0000E+00	2.2178E-03	3.4511E-03
N_2	0.0000E+00	0.0000E+00	2.7733E-03	3.5472E-03
CH_4	0.0000E+00	0.0000E+00	3.0737E-05	2.2516E-05

Appendix M   GTPRO simulation example

Figure M1 shows a print of the combined gas and steam cycle modeled in GTPRO. M is the mass flow in kg/s, T the temperature in K and p the pressure in bar.
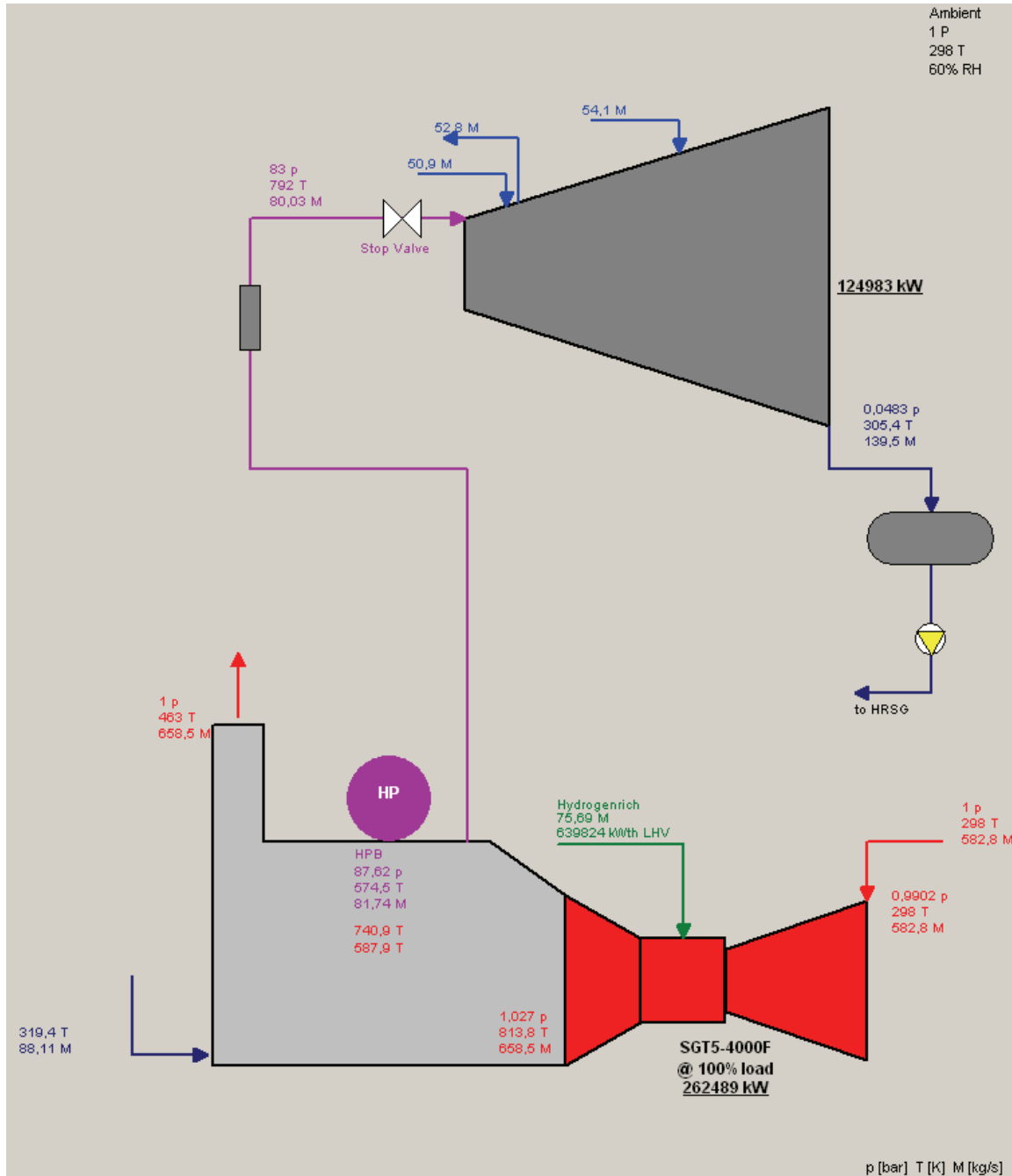

Figure M1. GTPRO print of a combined cycle.

Table M1 summarizes the calculations from the GTPRO simulation.

Table M1. Detailed results from GTPRO combined cycle simulation.

	Power Output kW		LHV Heat Rate kJ/kWh		Elect. Eff. LHV%	
	@ gen. term.	net	@ gen. term.	net	@ gen. term.	net
Gas Turbine	262489		8775		41,03	
Steam Turbine	124983					
Plant Total	387472	362763	5945	6350	60,56	56,7

PLANT EFFICIENCIES			
PURPA efficiency	**CHP efficiency**	**Power gen. eff. on**	**Canadian Class 43**
%	**%**	**chargeable energy, %**	**Heat Rate, kJ/kWh**
43,08	29,47	43,86	12672

GT fuel HHV/LHV ratio =	1,173	
DB fuel HHV/LHV ratio =	1,173	
Total plant fuel HHV heat input / LHV heat input =	1,173	
Fuel HHV chemical energy input =	750727	kW
Fuel LHV chemical energy input =	639825	kW
Total energy input (chemical LHV + ext. addn.) =	944109	kW
Energy chargeable to power (93,0% LHV alt. boiler) =	827128	kW

GAS TURBINE PERFORMANCE - SGT5-4000F					
	Gross power	**Gross LHV**	**Gross LHV**	**Exh. flow**	**Exh. temp.**
	output, kW	**efficiency, %**	**Heat Rate, kJ/kWh**	**kg/s**	**K**
per unit	262489	41,03	8775	659	814
Total	262489			659	

Number of gas turbine unit(s) =	1	
Gas turbine load [%] =	100	%
Fuel chemical HHV per gas turbine =	750727	kW
Fuel chemical LHV per gas turbine =	639825	kW

STEAM CYCLE PERFORMANCE				
HRSG eff.	**Gross power**	**Internal gross**	**Overall**	**Net process heat output**
%	**output, kW**	**elect. eff., %**	**elect. eff., %**	**kW**
68,5	124983	47,65	32,64	-174192

Number of steam turbine unit(s) =	1	
Fuel chemical HHV to duct burners =	0	kW
Fuel chemical LHV to duct burners =	0	kW
DB fuel chemical LHV + HRSG inlet sens. heat =	382946	kW
Net process heat output as % of total output =	-92,38	%

ESTIMATED PLANT AUXILIARIES (kW)		
GT fuel compressor(s)*	18074	kW
GT supercharging fan(s)*	0	kW
GT electric chiller(s)*	0	kW
GT chiller/heater water pump(s)	0	kW
HRSG feedpump(s)*	1504,9	kW
Condensate pump(s)*	257,7	kW
HRSG forced circulation pump(s)	0	kW
LTE recirculation pump(s)	0	kW
Cooling water pump(s)	850,4	kW
Air-cooled condenser fans	0	kW
Cooling tower fans	0	kW
HVAC	55	kW
Lights	100	kW
Aux. from PEACE running motor/load list	1004,8	kW
Miscellaneous gas turbine auxiliaries	464,8	kW
Miscellaneous steam cycle auxiliaries	266,7	kW
Miscellaneous plant auxiliaries	193,7	kW
Constant plant auxiliary load	0	kW
Gasification plant, ASU*	0	kW
Gasification plant, Coal mill	0	kW
Gasification plant, Other/misc	0	kW
Desalination plant auxiliaries	0	kW
Program estimated overall plant auxiliaries	22772	kW
Actual (user input) overall plant auxiliaries	22772	kW
Transformer losses	1937,4	kW
Total auxiliaries & transformer losses	**24709**	**kW**

* Heat balance related auxiliaries

PLANT HEAT BALANCE		
Energy In	**1090621**	**kW**
Ambient air sensible	14747	kW
Ambient air latent	17191	kW
Fuel enthalpy @ supply	756408	kW
External gas addition to combustor	0	kW
Steam and water	304284	kW
Makeup and process return	-2008,3	kW
Energy Out	**1091227**	**kW**
Net power output	362763	kW
Stack gas sensible	136243	kW
Stack gas latent	130777	kW
GT mechanical loss	1200,1	kW
GT gear box loss	0	kW

GT generator loss	3764	kW	
GT miscellaneous losses	1955,4	kW	
GT ancillary heat rejected	3398	kW	
GT process air bleed	0	kW	
Fuel compressor mech/elec loss	2711,1	kW	
Supercharging fan mech/elec loss	0	kW	
Condenser	289133	kW	
Process steam	148284	kW	
Process water	0	kW	
Blowdown	1158,4	kW	
Heat radiated from steam cycle	2613	kW	
ST/generator mech/elec/gear loss	2354,2	kW	
Non-heat balance related auxiliaries	2935,4	kW	
Transformer loss	1937,4	kW	
Energy In - Energy Out	**-605,4**	**kW**	**-0,0555** %
Zero enthalpy: dry gases & liquid water @ 32 F (273.15 K)			
Gas Turbine and Steam Cycle: Energy In - Energy Out = -605.4 kW			