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MODELING THE ENERGY INFRASTRUCTURE FOR ALBERTA'S OIL SANDS INDUSTRY: CURRENT TECHNOLOGY VS PETCOKE GASIFICATION

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What you need to invent is an imagination and a pile of junk (Thomas Edison)

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ABSTRACT

The exploitation of the Canadian oil sands is extremely expensive in terms of energy and cost. Alberta's oil sands companies extract bitumen and upgrade most of it to synthetic crude oil. During the upgrading, a large amount of petroleum coke is produced. Currently, this waste product is stockpiled, causing concerns on the possible effects for public health. In this work, petroleum coke gasification is evaluated as a source of energy for the processes.

Steam assisted gravity drainage (SAGD) method was selected for bitumen extraction. The technology considered for primary conversion of bitumen is thermal cracking and specifically delayed coking.

Once the streams energy demand is estimated, an energy infrastructure is created. In particular, a reference case (RC) and a gasification case (GC) are modeled with Aspen Plus. For both RC and GC the external fuel required and the CO_2 emissions are calculated. Additionally, a net energy analysis (NEA) was performed for each case.

The RC represents the current energy infrastructure of the oil sands industry. The results of the RC are then compared with the results obtained in similar studies.

In the GC, a gasification plant has been integrated in the energy infrastructure. The gasifier uses Shell's technology and is fueled with the petroleum coke generated from the bitumen upgrading. This plant produces electricity, steam and hydrogen for the processes. The GC is modeled both in CO_2 venting and carbon capture and storage (CCS) scenarios.

Upon modeling these two different systems, a comparative analysis is conducted which compares their performance and the emissions.

Keywords: Oil sands; Process modeling; Shell gasification; Polygeneration; Petroleum coke; Aspen plus simulation;

SOMMARIO

Lo sfruttamento delle sabbie bituminose canadesi risulta essere estremamente dispendioso dal punto di vista energetico ed economico. Le compagnie operanti nel settore estraggono il bitume dal sottosuolo e ne raffinano la maggior parte ad olio sintetico. Durante la raffinazione, viene prodotta una grande quantità di coke di petrolio. Attualmente, questo prodotto di scarto viene accatastato, causando preoccupazione per i possibili effetti negativi sulla salute delle persone. In questo studio, la gassificazione del coke di petrolio per la produzione di energia viene valutata come possibile alternativa al sistema attuale.

Sono stati considerati la tecnologia SAGD per l'estrazione del bitume dal sottosuolo ed il coking ritardato come metodo di conversione primaria del bitume.

Dopo aver calcolato la domanda di energia, è stato costruito un modello in grado di soddisfarla. In particolare, tramite l'utilizzo del software Aspen Plus, sono stati creati un caso base (RC) e un caso con gassificazione (GC). Per entrambi i modelli, sono state calcolate le emissioni di CO2. Sia per il RC sia per il GC inoltre, è stata effettuata un'analisi energetica chiamata *Net energy analysis (NEA)*.

Il RC è rappresentativo dell'attuale situazione nell'industria delle sabbie bituminose. I risultati ottenuti per il caso base sono stati confrontati con i risultati disponibili in letteratura da altri studi simili.

Nel GC, è stato integrato un impianto a gassificazione all'interno della struttura del RC, sostituendo parte delle tecnologie adottate precedentemente. Il gassificatore usa la tecnologia Shell ed è alimentato con il coke petrolifero generato dalla raffineria. Questo impianto produce elettricità, vapore e idrogeno per i vari processi. Per quanto riguarda il GC, è stato simulato anche uno scenario con cattura della CO₂ che riduce notevolmente le emissioni generate dall'impianto.

Infine, le prestazioni e le emissioni generate dai due scenari RC e GC sono state confrontate tra di loro e analizzate.

Parole chiave: Sabbie bituminose; Process modeling; Gassificazione Shell; Poligenerazione; Coke petrolifero; simulazione Aspen Plus;

ESTRATTO

Le sabbie bituminose dell'Alberta sono, dopo Arabia Saudita e Venezuela, la terza più grande riserva di petrolio del mondo. Esse consistono in un miscuglio di bitume, sabbia, argilla e acqua. Nonostante l'abbondanza nel sottosuolo, il recupero del bitume è particolarmente arduo e dispendioso energeticamente. Uno dei metodi più diffusi di estrazione del bitume in Alberta è la tecnologia di *Steam Assisted Gravity Drainage* (SAGD). La tecnologia SAGD prevede la perforazione di due pozzi orizzontali nel sottosuolo. Una gran quantità di vapore saturo ad alta pressione viene continuamente iniettata attraverso il pozzo superiore. Il vapore acqueo forma una "camera di vapore" che cresce orizzontalmente e verticalmente nella formazione. Il vapore scalda il bitume e ne riduce la viscosità, condensando a propria volta e costringendo il bitume a defluire nel pozzo inferiore per gravità. Nel pozzo inferiore sono installate delle pompe sommerse che portano il bitume in superficie, assieme ai gas disciolti in esso e all'acqua condensata. I diversi fluidi vengono in seguito separati attraverso un trattamento altrettanto dispendioso energeticamente.

Per quanto detto dunque, l'estrazione del bitume dal sottosuolo necessita di un input energetico estremamente elevato dall'esterno, sotto forma di vapore ed energia elettrica.

Il bitume estratto è un prodotto ancora estremamente grezzo e pesante. Le normali raffinerie di petrolio non possiedono le caratteristiche necessarie per poterlo raffinare e per produrre combustibili liquidi commerciali. Per rendere questo prodotto competitivo sul mercato è richiesta un raffinazione intermedia. Il risultato della raffinazione intermedia è chiamato olio sintetico e possiede caratteristiche simili ai crudi leggeri.

La raffinazione intermedia consiste solitamente in un cracking termico ad alta temperatura a cui segue un'idrogenazione dei prodotti liquidi in *hydrotreaters* per rimuovere solfo e composti azotati.

La raffinazione intermedia richiede anch'essa grandi quantitativi di energia, sotto forma di idrogeno, elettricità e vapore.

E' chiaro dunque che il processo di estrazione del bitume e la sua raffinazione ad olio sintetico consumino quantitativi di energia primaria estremamente elevati.

A causa delle altissime emissioni di anidride carbonica , le *oil sands* da sole sono il più grande emettitore di gas serra di tutto il Canada. Per questo motivo il governo canadese da tempo cerca di limitare le emissioni legate a questa attività tramite penalità sulle emissioni. Dal 2007 è in vigore una norma che prevede la riduzione del 12% delle emissioni di CO_2 rispetto ai valori del 2005.

Il coking ritardato è il processo di cracking termico più diffuso nell'industria delle *oil sands*. Ad onor del vero, questo processo non è affatto il più efficiente in commercio.

Tuttavia, esso risulta di gran lunga il processo più economico, ad oggi, per la raffinazione del bitume in Nord America.

Il principale problema legato a questo processo è l'ingente quantità di coke di petrolio generato. Il coke di petrolio delle *oil sands* canadesi contiene grandi quantità di zolfo e metalli pesanti. Per questo motivo, risulta impensabile una sua combustione diretta, che causerebbe elevatissime emissioni di SO₂. L'alto quantitativo di zolfo non rende attrattivo nemmeno l'uso del petcoke nell'industria elettrochimica. Come conseguenza, da anni il *petcoke* delle *oil sands* viene stoccato in superficie. Recentemente, le immense montagne di *petcoke* sono arrivate fino ad alcuni centri urbani, destando preoccupazione nell'opinione pubblica.

In questo studio è stata effettuata un'analisi approfondita dell'infrastruttura energetica attuale delle *oilsan*ds, valutandone i consumi e le emissioni di CO₂. Si è cercato poi di fornire una soluzione sostenibile dal punto di vista energetico e ambientale, che consenta in modo efficiente lo smaltimento del petcoke, riducendo il consumo di gas naturale nonché le emissioni di CO2 legate allo sfruttamento delle *Oil Sands*. Il lavoro è diviso in quattro capitoli:

Nel primo capitolo è trattato lo stato attuale delle sabbie bituminose canadesi. In particolare, gran parte di questo capitolo è dedicata a una spiegazione di carattere generale sulla tecnologia di estrazione e raffinazione del bitume.

Nel secondo capitalo è stata calcolata la domanda energetica per i processi di estrazione e raffinazione. Per quanto riguarda il processo SAGD, le equazioni necessarie a descrivere il modello hanno una struttura piuttosto semplice, che prevede l'utilizzo di pochi parametri atti a calcolare la domanda energetica *(SOR, EOR, GOR).* Tuttavia, al fine di selezionare un *range* di valori adeguato per questi parametri, sono stati usati studiati un gran numero di impianti operativi in Alberta. Dopo aver analizzato i parametri di funzionamento dei suddetti impianti, è stato selezionato il *range* di valori opportuno.

La previsione della domanda per il processo di raffinazione ad olio sintetico è stata invece decisamente più complessa. Innanzitutto, è stato necessario creare un modello semplificato di raffineria costituito da diverse unità (separazione del diluente, coking ritardato e *hydrotreaters* per le diverse frazioni liquide). In seguito, è stato necessario l'ausilio di correlazioni presenti in letteratura per (i) calcolare le frazione idrocarburiche prodotte dalle unità e poter stabilire i flussi di massa coinvolti nei processi (ii) calcolare la domanda di elettricità, idrogeno, vapore e combustibile richiesta dalle diverse unità della raffineria. Questo modello semplificato per la raffinazione del bitume ha portato alla produzione di un flusso di olio sintetico con le specifiche solitamente richieste dalla raffineria a valle. Il calcolo della domanda di energia ha evidenziato una grandissima richiesta di vapore da parte dell'estrazione SAGD, che risulta di gran lunga il flusso energetico più elevato. La richiesta di idrogeno risulta consistente, specialmente a causa degli elevati contenuti di zolfo nei prodotti liquidi del cracking. La domanda di elettricità risulta invece più modesta

rispetto agli altri flussi energetici. Infine, è doveroso ricordare come le unità stesse della raffineria richiedano una grande quantità di combustibile per riscaldare i flussi in ingresso ai reattori.

Una volta che la domanda di energia è stata calcolata, è stato costruito un modello in grado di soddisfarla. In particolare, sono stati creati un caso base e un caso con gassificazione di petcoke petrolifero, tramite l'utilizzo del software Aspen Plus.

Il capitolo 3 è interamente dedicato alla descrizione del modello per il caso base. Il caso base è rappresentativo dell'attuale situazione nell'industria delle sabbie bituminose. L'infrastruttura energetica è stata costruita in rispetto alle particolarità delle imprese operanti in Alberta. Il combustibile utilizzato nel caso base è quasi esclusivamente gas naturale prelevato dalla rete.

Nel caso base, sono state usate turbine a gas alimentate a gas naturale per la cogenerazione di energia elettrica e vapore. Nell'impianto cogenerativo, è stato creato un modello di caldaia a recupero con postcombustione dei gas di scarico. La domanda di vapore è stata soddisfatta tramite l'uso di due tecnologie: (i) evaporatori OTSGs alimentati a gas naturale per il vapore richiesto dal processo SAGD e (ii) caldaie a corpo cilindrico alimentate a gas naturale per il vapore richiesto dalla raffineria. Per produrre l'idrogeno necessario, è stato creato un modello di impianto di *Steam reforming* di gas naturale, il quale produce anche del vapore in eccesso utilizzabile nella raffineria. I risultati ottenuti per il caso base sono stati confrontati con i risultati disponibili in letteratura da altri studi simili. Il caso base ha fornito risultati del tutto comparabili con quelli dei modelli presenti in letteratura

Nel caso con gassificazione, è stato integrato un impianto poligenerativo all'interno della struttura del caso base, sostituendo parte delle tecnologie adottate precedentemente. Il gassificatore usa la tecnologia Shell ed è alimentato con il coke petrolifero generato dalla raffineria. Il gassificatore produce gas di sintesi, che può essere convertito ad idrogeno puro o essere utilizzato come combustibile in turbine a gas. L'impianto poligenerativo inoltre, può generare una discreta quantità di vapore, grazie al calore disponibile dal raffreddamento del *syngas*.

Il modello di sistema poligenerativo soddisfa l'intera domanda di idrogeno e di vapore della raffineria attraverso la conversione del syngas ed il calore disponibile dai *syngas coolers*. Il gas di sintesi rimanente viene invece utilizzato in turbine a gas per cogenerare elettricità e vapore. L'elettricità viene utilizzata nei processi e dagli ausiliari, mentre il vapore cogenerato viene iniettato nei pozzi SAGD.

Per il caso con gassificazione, sono stati effettuati due modelli differenti:

- Caso con emissioni di CO₂ in atmosfera
- Caso con cattura di CO₂ dal gas di sintesi e sequestro in giacimenti esausti

L'obiettivo principale è stato quello di creare un modello che utilizzasse in maniera efficiente il petcoke prodotto dalla raffineria e allo stesso tempo permettesse una riduzione delle emissioni di gas serra in atmosfera.

La comparazione dei due casi ha evidenziato che è possibile fare un uso efficiente del petcoke. Dal punto di vista energetico, questa soluzione si può definire ideale, in quanto si riducono di gran lunga gli input di energia primaria dall'esterno. L'utilizzo del petcoke come combustibile principale permette di ridurre in maniera importante l'utilizzo di gas naturale.

D'altra parte, l'alto contenuto di carbonio del coke di petrolio innalza notevolmente le emissioni di CO_2 , rispetto al caso base. Per questo motivo, la cattura di CO_2 è indispensabile per rendere accettabile questa tecnologia.

La gassificazione del petcoke con cattura di CO2 potrebbe essere una soluzione sostenibile dal punto di vista energetico e ambientale. Inoltre, consentirebbe lo smaltimento del petcoke in modo efficiente, riducendo anche il consumo di gas naturale nonché le emissioni di CO2 legate allo sfruttamento delle *Oil Sands*.

CHAPTER 1: Introduction

1.1 THE OIL SANDS INDUSTRY

Canada, with its 173 billion barrels, has the third largest oil reserves in the world, after Saudi Arabia and Venezuela.

According to the latest reports [1], 170 billion of these barrels are located in Alberta and 168 billion of them are recovered from bitumen. This resource has always been well known but is now gaining attention as conventional supplies continue to be depleted. These numbers refer to the bitumen that is possible to extract economically with current technology. With new technological improvements, the reserve estimate could be significantly higher. In fact, the total reserves in place are estimated to be around 1.8 trillion barrels [1].

Accordingly to the Spring 2015 update of Alberta's oil sands industry [1], more than 2 million bbls/d of bitumen were produced in September 2014 from the oil sands. These numbers are impressive and make Canada the fifth largest producer of oil in the world [2]. Nevertheless, the extraction of bitumen from the oil sands industry is particularly energy intensive. Bitumen is a very heavy form of petroleum with a very high viscosity. Alberta's oil sands companies extract bitumen and upgrade most of it to synthetic crude oil (SCO), which has characteristics similar to the conventional light crudes. In the extraction and upgrading processes, a large amount of energy in the form of steam, electricity and hydrogen is consumed. This energy is produced using hydrocarbons, which contributes to significant CO₂ emissions. The CO₂ emissions from energy production for bitumen extraction and upgrading to SCO are estimated to be 18-41 gCO₂eq/MJ SCO (comprising direct and indirect emissions) [3]. Due to these very high emissions, Canadian oil sands are by far the single largest contributor to greenhouse gases (GHG) emissions in Canada. [4] The concerns about emissions, along with the low price of natural gas, switched the fuel choice to lower carbon fuels.

However, in 2007 Alberta introduced reduction objectives of 12% on CO₂ emissions for all the plants emitting more than 0.1 Mt CO₂/year. New plants have a reduction target of 2% from the fourth year of operation, which increases by 2% annually up to 12%. The facilities can improve their performance or can pay carbon taxes for emissions beyond the mandatory target [5]. Since all the plants in the oil sands industry use high efficiency natural gas fueled facilities for energy production, it is very difficult to further reduce the emissions of CO₂. Because of that, rigorous investigation is being conducted on carbon capture and storage (CCS) technology.

However, the CO_2 emissions are not the only environmental problem connected to the oil sands industry. As mentioned, the bitumen extracted from the subsoil needs to be upgraded to SCO in order to meet the characteristics of the conventional light crudes.

Most of the companies upgrade the bitumen with thermal cracking. Although this technology is very cost effective, it produces large amounts of petroleum coke as a by-product.

The petroleum coke (petcoke) contains in high quantity practically all the environmental negative components originally in the bitumen. Due to the presence of sulphur and heavy metals, a direct combustion of the petcoke has always been considered impractical [6]. Despite its high heating value, the petcoke use as a fuel (fuel grade coke) has always been considered very unattractive.

On the other hand, fine petcoke can be used as a source of carbon (anode grade coke) in the electrochemical industry. In general, anode grade petcoke should have a molar fraction lower than 3% [6]. Since the oil sands petcoke usually has a content of sulfur from 5-7 % mol, it cannot be considered an ideal anode grade coke.

As a result, the petcoke produced in the oil sands is stockpiled. Over time, the petcoke started to create real mountains in Alberta (Figure 1). In the recent period, petcoke from oil sands bitumen refined in the US started to accumulate dangerously in big cities such as Chicago and Detroit. These 'petcoke emergencies' have appeared in newspapers and captured the public attention, causing big concerns on the possible effects for public health. It is clear that stockpiling is not a solution to this problem.



Figure 1: Mountain of petroleum coke in Alberta

The only possible use of the petcoke seems to be through a gasification process. Gasification technologies have become a mature and reliable alternative for solid fuels exploitation. According to Furimsky [7], both Shell and Texaco guarantee that oil sands petcoke can be an ideal feedstock in their entrained bed reactors.

A gasification based poligenerative plant can be used to produce steam, electricity, and hydrogen for the processes of bitumen extraction and upgrading to SCO.

The idea of using the waste product of the oil sands as the main fuel for their exploitations seems to be very interesting. Unfortunately, gasification of petcoke generates by far more CO_2 emissions than natural gas combustion.

However, gasification also provides some of the least costly methods for large scale CO₂ capture for sequestration in deep geologic formations away from the atmosphere. [8] Petcoke gasification with CCS can combine the use of an undesirable and problematic waste product with a reduction in GHG emissions to the level required by the government.

1.2 ALBERTA'S BITUMEN RECOVERY

The main ways to extract bitumen from the underground are *surface mining* and *in situ* recovery.

The former method is mainly used to extract bitumen from shallow mines and it is limited to areas where the total overburden does not exceed 75 m. With this technology, the muskeg and the overburden are removed to expose the oil sand deposit and collect the material with shovels and trucks.

The oil and sand mixture is then broken into small pieces and transported to extraction facilities where is separated with hot water and soda or kerosene and chemicals [9]. Although surface mining is a simple process used to extract bitumen, it can only access around 20% of the recoverable bitumen in Alberta because the remaining 80% is too deep to be extracted with this technology.

The second extraction method, *in situ* (from Latin, in place), uses wells instead of trucks and shovels to extract the bitumen from the underground.

Because of the characteristic of the bitumen (it is semi-solid with really high viscosity) it needs to be heated and fluidized to be recovered.

The main commercial methods of *in situ* extraction are Cyclic steam simulation (CCS) and steam assisted gravity drainage (SAGD).Both of these methods use high pressure steam to enhance the oil recovery.

In CCS the steam is injected into wells drilled from pads for a period of time, then the steam is left to soak and melt the bitumen in the reservoir and the same wells are switched into production mode bringing the bitumen to the surface.

In SAGD two parallel horizontal wells are drilled from the surface for continuous steam injection and fluid production. The steam is injected in the top well and forms a steam chamber, heating the bitumen and melting it (Figure 2). The melted bitumen and the condensed water are forming an emulsion that is artificially lifted to the surface and properly treated

SAGD is the most important *in situ* method used while CCS has just few applications in the area of Cold Lake and Peace River deposits [1].



Figure 2: Scheme of a SAGD process

Research is underway on a number of other methods or variations of *in situ* extraction such as *in situ* combustion, polymer or CO_2 injection, Vapex or Thai methods, but none of them is actually operative.

In this study, the SAGD technology is the only one considered, because it is the most often employed method that has greater potential for the future.

In 2012 for the first time *in situ* production exceeded surface mining in Alberta where 53% of the oil sands production was provided by *in situ* technologies.

Because of the reliability and the maturity of SAGD technology, this percentage is expected to grow in the future making SAGD the market leader in Alberta's Oil sand extraction.

1.3 STATUS OF THE MARKET

North Athabasca, South Athabasca, Cold Lake and Peace River are the areas in Alberta where bitumen is extracted with SAGD method (Figure 3)

In North Athabasca, Suncor is the main leader with Firebag and Mckay River plants (218500 bbl/day) with 92% of the market share.

In the comingyears, many companies will start to invest and operate in this region, bringing the production levels to 1122500 bbl/day in 2020(a growth of almost 400%) and making the market more heterogeneous and competitive.

In south Athabasca the production of bitumen is more mature and will almost double in 2020 from 666700 bbl/day to 1897400 bbl/days.

The leading actor in this region is Cenovus Energy with plants in Foster Creek and Christina Lake(304000 bbl/day) which are guaranteeing the 45% of the market share now and 35% in 2020.



Figure 3: Map of the Oil sands area

In North and South Athabasca many important companies like Conocophillips, Devon Canada, Meg energy, Husky, Brion Energy and Canadian Natural Resources plan to have more than 100000 bbl/days SAGD plants installed by 2020. This confirms the maturity of, this technology and the high level of interest that it has garnered. [1]

The areas of Cold Lake and Peace River have a smaller production of bitumen mainly with the CCS technology.

The Cold Lake area has a production of around 270000 bbl/day mainly from the Canada Natural Resources and Imperial Oil CCS extraction plants installed in 1985 and still operative. Those two plants are not planned to be expanded and will remain the main market leader in this area although some small-medium size plants will be installed by other companies in this area.

The Peace River area has a small production of bitumen (around 16000bbls/day). In this area, Royal Dutch Shell will be the main actor in the future with its VSD (vertical Steam Drive) plant of 92500 bbls/day.

Globally Alberta's Oil sands are producing almost 1200 thousands of bbls/day with *in situ* methods. In 2020 they are expected to produce around 3500 thousands of bbls/day with an incredible growth of 190%.

The total scheduled capacity of installation will be 6200 thousands bbls/day which is more than five times the current production.

These numbers are forecasting an impressive growth in the *in situ* bitumen production that will be a very important actor in the future economy of Canada.

The massive investments in this sector will bring improvements in the technology and an overall reduction in costs.

All these data are taken and then elaborated on a calculus sheet from the 2014 fall quarterly update of Alberta oil sands industry [1].

The results are shown in Figure 4.

In the calculations, It has been assumed that the planned capacity expansion in the oil sands industry will be concluded between 2020 and 2030.

The investment for which the specific capacity is not indicated in the report [1] are not counted because are considered still in phase of evaluation.



Figure 4: Oil sands forecast production

1.4 SAGD PROCESS TECHNOLOGY

1.4.1 Steam injection

In a SAGD process a two pair of horizontal wells is drilled from the surface.

The lower one or production well is drilled just 1 or 2 m above the SAGD base while the upper one or injection well is drilled on the top of the reservoir. The distance between the two pipes is usually 5 meters.

The pair wells can reach a depth of 200-800m, depending on where is the target reservoir located.

Steam injection generates a high temperature vapor chamber that heats the surrounding bitumen, allowing it to drain by gravity into the lower well (the production well) [10] The amount of high pressure steam injected in the reservoir vary widely from one project to another and the parameter that synthesize better the amount of steam required is *the* Steam Oil Ratio (SOR) that is measured in m3 water/m3 bitumen CWE (Cold Water Equivalent) and will be explained in more details in the next sections.

1.4.2 Enhanced lift

The steam, after rising and melting the bitumen, condenses and forms an emulsion with the bitumen that is sent to the ground facilities with an artificial lift.

There are mainly two ways of lifting the emulsion. In gas lift, non-condensable gases are compressed and injected in the underground with steam. The other way to lift artificially the emulsion is using downhole electrical submersible pumps(ESPs).

Gas lift has always been used because of its simplicity and reliability. In this configuration the gas produced from the wells is compressed and injected into the steam chamber.

The main disadvantages of gas lift are the electricity consumption of the compressors and the necessity of a high steam chamber pressure for the gas lift [11].

The benefits of using low pressures in the steam chamber are completely clear and the advantages of ESPs are evident and demonstrated in the literature [12].

Although in the first SAGD plants gas lift was the most used technology, now most of the companies (like Cenovus and Suncor) have almost totally replaced it with ESPs.

1.4.3 Separation and De-oiling

Once the emulsion arrives on the surface the separation of the different components takes place at the central processing facility (CPF) of the SAGD plants.

The complete scheme of the CPS is shown in Figure 5.

The emulsion is generally composed of water, heavy bitumen and solution gas.

Not just the oil but all of these products are really important and precious into the SAGD plant, each one for different reasons. The SAGD extraction is a water intensive process and water is a scarce resource in Alberta; the reason why it should be recovered as much of water as possible. The produced gas instead, can be used after proper treatment as a fuel and can contribute to reducing the consumption of natural gas.

The first surface facility is called degasser and separates the solution gas from the rest of the emulsion. This unit is a vessel that separates the gas from the liquid through a flash separation.

After the degasser the emulsion enters into free-water knock outs (FWKOs). The FWKO is a three phase separation system consisting of a horizontal vessel that separates the different phases mainly by gravity. This unit is separating most of the water, which is sent to the deoiling. The emulsion separation general scheme is shown in Figure 6.

The bitumen, which still contains a consistent amount of water is fed into electrostatic treaters to remove the remaining water.

The gas that is produced into these three units (degasser, FWKO and treaters) is sent to the vapor recovery unit (VRU).

The emulsion coming out from the wells, thanks to presence of the water and to the temperature has a lower viscosity than the bitumen itself. Before each of those



Figure 5 : Central Processing Facility complete scheme from [13]

separation steps, a certain amount of diluent is added (typically naphtha) to make the separation easier. This addition of diluent permits to lower the viscosity of the bitumen when the stream is cooled down.



Figure 6: Emulsion separation

After the separations the water is de-oiled. The de-oiling process is shown in Figure 7. De-oiling consists mainly of skim tanks, induced gas flotation (IGF) and oil removal filters (ORFs) units.

The skim tank is a simple big tank that separates water from oil by gravity.



Figure 7: Water de-oiling

The IGF is a horizontal tank where some gases (typically N_2) are introduced into the emulsion. The bubbles adhere to the suspended matter making it float on the water surface where it can be easily removed. The ORFs are walnut shell filters.

All the oil and the gas that is recovered from those processes is sent respectively into the oil recovery unit and the vapor recovery unit (VRU).

1.4.4 Water Softening

Once the water is de-oiled it needs to be softened to reach the specification required from the steam generators.

Warm lime softeners (WLS) and evaporators are the two main technologies used in water softening.

In WLS, chemicals like lime and MagOx are introduced into the feed water. The chemicals react with the harnesses of the water and remove most of the silica within it. The WLS produces a water that still contains some harnesses. Because of this it is mandatory to use once through steam generators (OTSGs). These boilers are more resistant to harnesses than drum boilers, but produce steam with a maximum quality of 80%. This fact make the OTSGs less efficient compared to drum boilers and requires a separator before the injection in the produced wells.

A plant with WLS can hardly reach a rate of recycled water larger than 90%. The other water should be sent to disposal.

Evaporators consists of big shell and tube towers. They work with the vapor compression principle. The flowsheet scheme of evaporators is shown in Figure 8. The liquid is entering into the evaporator tower from the top through a high number of pipes. Meanwhile the water falls down into the pipes due to gravity, it is heated and starts to evaporate. The vapor is dragged down to the bottom of the tower by the water. The steam then flows into a compressor where there is enhanced pressure. Generally speaking, compression of steam enhances both pressure and temperature.

The high pressure steam is then sent back to the evaporator shell where it heats the liquid into the pipes. The high pressure steam, while it is exchanging heat is condensing, producing a high quality distillate.

In this way no external heat is required. The external energy for the evaporation/distillation is just the electricity consumed by the compressor.

The liquid not evaporated from the pipes, called brine, is recirculated to the top several times. Part of the brine is sent to another unit called crystallizer that essentially evaporates the liquid water content of the brine by using part of the heat of the high pressure steam exiting the compressor. The waste product is almost solid and in some cases can be sold as a byproduct. [14]

With evaporators it is possible to produce a water much more pure and to reach recycle rates close to 100% achieving what is called zero liquid discharge (ZLD). Evaporators furthermore make possible the use of drum boilers, that are more efficient and economic. On the other hand, this technology is more energy intensive than WLS and results in higher operating costs and higher emissions.

This happens primarily because the electricity required to operate the compressors is superior than the other energy usage savings. [12].

Typically a solution like an evaporator can increase the emissions between 3 and 10% in an overall SAGD plant [15].



Figure 8: Evaporator general scheme from [14]

Although evaporators with drum boilers seems to be a more advanced solution to soften water and to reach higher recycle rates, many studies have demonstrated that their application is still not convenient and much more expensive than the WLS with OTSGs. Nevertheless, there are situations where the saving of water can be more important than the saving of energy(Section 2.1.5). A good configuration involves the installation of an evaporator for the liquid product separated after the OTSGs maintaining WLS as the main softening technology. This permits to achieve ZLD with a smaller unit or less units. With that configuration the increase of electricity consumption can be limited, while nowadays the installation of evaporators as the main softening technology seems to be impracticable. The ZLD technology on blowdown has been successfully installed on Suncor Mckay SAGD plant.

1.4.5 Vapor Recovery unit and Sweetening

During the process of separation there is a certain amount of vapors that is released and recovered from a VRU.

Those vapors are mainly produced in the FWKO and in some tanks of the CPF. The recovered vapors, together with the non-condensable gases of the solution gas separated in the degasser, are mixed and sent to an Acid Gas Removal (AGR) Unit. This happens because there is a certain concentration of H_2S in the gas that can produce SO_2 during the combustion.

Sulphur Inlet Rate (tonnes/day)	Design Sulphur Recovery Criteria (%)	Calendar Quarter-Year Sulphur Recovery Guidelines (%)
< 1	none required	none required
1 to 5	70	69.7
>5 to 10	90	89.7
>10 to 50	96.2	95.9

There is a certain requirement of purification depending on the SO₂ emissions of a plant (Figure 9). For plants that emit less than 1 ton SO₂/day desulphurization is not mandatory.

Figure 9 : Sulphur recovery criteria in Alberta's Oil Sands from [16]

The produced gas and vapors are sent to a column where the acid gases are absorbed from a solvent. The type of absorption can be chemical or physical.

One of the most used technology in gas de-sulphurization is the Shell Sulfinol process. This process is used in Athabasca region for example by Suncor [17]. This technology is combining the advantages of physical and chemical absorption and is using as a solvent a mixture of sulfolan, water and MDEA (methyl-diethanolamine).

The solvent rich of acid gases is sent to a stripping column where the acid gases are separated from the solvent with water. The acid gases are separated and sent to a Claus facility while the solvent is regenerated in a reboiler and sent back to the absorption column (Figure 10).



Figure 10: Flow diagram for a conventional AGR unit

Once the gas has been cleaned up it is sent to a mixing unit where is mixed with low pressure natural gas and sent to the mix-fuel OTSGs.

1.4.6 Steam generation

Once the water is softened and integrated with clean make up water it is sent to the boiler feed water (BFW) tank and after to the steam generators.

As previously discussed, drum boilers can be used only with evaporators, and because of that the most used steam generators are OTSGs.

This type of steam generator can be fueled either with solid or gaseous feeds, and to evaporate water that is not necessarily very clean.

Because of the Canadian government's severity on CO₂ emissions, only fuel gases are typically used (natural gas and sweet produced gas).

Another way to generate steam that is becoming important in SAGD plants is cogeneration in a once through heat recovery steam generator (OT-HRSG)

This solution is only possible if the plant is producing electricity with its own gas turbines (GT). The exhaust gases of the GT are typically posfired and used in a OT-HRSG to produce steam with characteristics similar to the one of the OTSGS.

After the separation, the steam is finally sent to the wells while the liquid can either be recycled in the water treatment, used in another stage of OTSG or sent to disposal.

1.4.7 Heat exchangers system

The process previously described uses an efficient system of heat exchangers.

The emulsion from the wells surfaces with a temperature of 170-180°C but needs to be cooled down for water de-oiling.

The plant uses a complex system of heat exchangers that permits the recovery of almost all the heat that would be lost in the de-oiling processes. The recovered heat preheats the BFW.

Thanks to this exceptional system of heat exchangers, the water reaches a temperature of around 160-170°C. This value is just 10-15 °C lower than the temperature of the emulsion entering the CPF. The blow down of the OTSGs is at a high temperature that preheats the BFW till a value around 200 °C.

There is a glycol system of heat exchangers that recovers heat from many parts of the CPS and provides it where required. The main goal of the glycol system is to preheat the air of the burners and to heat the offices of the employees.

If for any reason, the glycol system won't reach the required temperature, a NG backup boiler will be turned on.

1.5 UPGRADING PROCESS TECHNOLOGY

1.5.1 Bitumen, dilbit and SCO

The bitumen of Alberta's oil sands is a product with an extremely high density (8-10°API) and very high viscosity.

The characteristic of oil-sands bitumen, compared with conventional light and medium gravity oil, are provided by Meyers [18]:

- Extremely high viscosity at ambient temperatures that makes pipeline transportation impossible without the addition of a substantial amount of diluent such as natural gas condensate or naphtha.
- Deficiency of hydrogen compared with the hydrogen content of conventional light and medium-gravity crude oils.
- Large percentage of high-boiling-point material which limits the volume of virgin transportation fuels that may be recovered by simple separation processes.
- Substantial quantities of resins and asphaltenes which act as coke precursors in high-temperature refining operations.
- High content of sulphur and/or nitrogen content, which requires severe hydroprocessing of the distillate fractions to produce fuels or intermediate products for refineries

Property		Bitumen	Synthetic Crude Oil	Crude Oil
Gravity, °API		8	32	35
Sulfur, % w/w		4.8	0.2	0.1
Nitrogen, % w	/w	0.4	0.1	0.2
Viscosity, cent	tipoise at 100°F	500,000	10	10
Distillation pro	ofile, % w/w (cumulative)			
°C	°F			
0	30	0	5	5
30	85	0	30	30
220	430	1	60	40
345	650	17	90	70
550	1020	45	100	90
Residuum		100		100

Properties of Synthetic Crude Oil from Athabasca Bitumen

Figure 11: Comparison of Some properties of Bitumen, Synthetic Crude and Light Crude

The comparison of some characteristics of bitumen, SCO, and a conventional light crude oil are shown in Figure 11.

As was mentioned before, due to the high viscosity of the bitumen, it is impossible to transport it in pipelines. Because of this reason, diluents is added to lower the density and the viscosity. The product, called dilbit, can be easily transported in pipelines.

The dilbit has two main ways of being refined. The first option is to send it directly to a refinery, where the diluent is sent back to the SAGD plant and the bitumen is refined to finished products for customers.

The second one is to upgrade it close to the SAGD plant to an intermediate product called synthetic crude oil (SCO) and then send it to the refineries.

The last option is the preferred one, for a specific reason:

Most of the refineries used to handling light crude oil and are not equipped to refine such heavy oils like Alberta's bitumen. This happens especially in the US, which is one of the main markets for oil sands companies.

During the processes of upgrading, most of the undesirable components of the bitumen, like sulphur and heavy metals, are reduced.

Moreover, the SCO contains molecules with less atoms of carbon and less aromatics rings. Those characteristics makes the SCO a competitive and desirable product for the refinery market.

1.5.2 Types of Cracking

Coking and hydrocracking are the two main ways for cracking and upgrading the bitumen to SCO.

Coking is a non catalytic thermal cracking process based on the concept of carbon rejection. The heaviest and carbon deficient portions of the feed, like resins and asphaltens, are rejected as coke. [9]

The coke contains the majority of the sulfur and nitrogen and almost the entire metals of the feedstock.

Hydrocracking adds hydrogen to crack the molecules and make a lighter product. Hydrocracking usually produces SCO with increased liquid fraction yields and lowersulphur products, but it is more expensive for the massive amount of hydrogen demanded. Although many companies have started to use hydrocracking for the bitumen upgrading,

thermal cracking is principally used in the oil sands industry.

In the oil sands industry, there are some different processes for thermal cracking as delayed coking, fluid coking and Flexxicoking.

The first technology has a lower conversion to SCO and produces less liquid and gas products than the other two. This technology produces much more coke than any other process. Despite these disadvantages it is simple and economical.

Suncor, the biggest producer in the SAGD oil sands industry, uses delayed coking. Furthermore, as will be explained in the next sections, it is possible to use the petcoke as the main fuel for the entire process with gasification. In that case, the massive presence of petcoke will be a resource and not a problem.

Due to all these reasons, delayed coking is selected as the upgrading process for this study. The general scheme for the bitumen upgrading is shown in Figure 12.

1.5.3 Diluent recovery Unit

The first unit of the upgrading process is the diluent recovery unit (DRU).

The DRU is essentially a column of distillation where the diluent is separated from the bitumen and sent back to the CPF of the SAGD process.

In this unit there is also a certain separation of light gas oil. In the DRU, although almost all the diluent is recovered, there are a few losses that necessitate a small make up of diluent. According to the work of Ordorica-Garcia [19], 98% of the diluent is recovered in this unit.

The residue, called atmospheric topped bitumen (ATB) is sent to the delayed coker. Some upgrading plants install also a vacuum distillation unit before the thermal cracking that can handle all the ATB or part of it.

This configuration increases the production of lighter fractions (and consequently the quality of the SCO), but at the same time enhances the consumption of energy. Because of that, the installation of a VDU should be evaluated case by case.



Figure 12: General Scheme for the Upgrading process

1.5.4 Delayed Coker

The delayed coking process is based on a semi-continuous batch bed.

The process consists of an empty drum where the thermal decomposition of hydrocarbons occurs.
The coke produced during the reaction is deposited into the drum; meanwhile, the light hydrocarbons are sent to a fractioning column where they are separated into the different products. The scheme of the process is shown in Figure 13.

The delayed coker process has at least two coke drums that are alternating in cycles of 24-48 hours so that one drum is in its coking cycle while the other one is in the regenerating cycle.

When one drum is filled with coke, it is switched to a cooling and decoking cycle and the other drum is placed in coking service [9].

Most of the plants use a hydraulic system for decoking. This system consists in a number of high pressure water jets which are lowered into the coke bed on a rotating drill stem [20]. The coking process is totally insensitive to the feedstock quality and its content of metals, sulphur, nitrogen and asphaltanes.

Thanks to that characteristic, it can perfectly handle the atmospheric topped residue that is the feedstock of the process. According to Huc [9], typical reactor yield data are:

- 10-13 wt% gas product
- 60-70 wt% total liquid product
- 20-30 wt% reactor coke



Figure 13: Delayed Coking scheme process from [9]

The feedstock is usually preheated and sent to the bottom of the fractioning tower, where it is accumulated before the furnace.

In the furnace the stream is heated by the combustion of fuel gas to around 480-515°C. This is the temperature at which thermal cracking usually takes place.

It is very important to avoid coke deposition into the furnace, and because of that the residence times in the furnace should be short and the velocity of the stream high. In order to do that, high pressure superheated steam is injected. The steam injected

enhances the velocity and shortens the residence time of the feed into the furnace by pushing it into the coke drum.

In the coke drum the endothermic cracking reaction occurs and the coke is deposited at around 414-465°C.

The light hydrocarbons are sent into the fractioning tower that divides them into different streams.

- Overhead sour gas, which needs to be de-sulfurized before use as a fuel
- Naphtha
- LGO
- HGO

The main residue is the petcoke, which contains a big amount of nitrogen and sulphur and almost all the nickel, ash and vanadium.

The coke which falls from the drum is usually collected in trucks.

1.5.5 Hydrotreater

All the liquid distillates coming from the delayed coking are very high in diolefin, olefin, nitrogen and sulphur content. Consequently, all the liquid products should be further refined to meet the product demand.

In order to eliminate the impurities and reach the required specification a severe hydrotreatment is mandatory.

During the hydrotreatment, the liquid distillates enter in a reactor where a significant amount of hydrogen is provided, in order to hydrogenate some molecules. The aim of the hydrotreatment is to:

- Reduce the concentration of impurities such as sulphur and nitrogen to levels suitable for downstream refining to finished products
- Saturate olefins and diolephins into more stable paraffinic and naphtenic structures
- Saturate some aromatic rings to lower rings structures and to naphtene in order to produce the required diesel cetane number for the diesel fraction and the required jet fuel smoke point.

Three hydrotreating units should be considered in a bitumen upgrading plant:

- Naphtha hydrotreatment unit
- Diesel/jet hydrotreatment unit (aromatic saturation unit)

• Heavy coker gasoil hydrotreatment or hydrocracking

1.5.6 Acid gas removal

The H_2S rich off gas from hydroprocessing is combined with the off gas produced in the other units and processed in an AGR, similar to the unit described in the SAGD process. The hydrogen sulfide is removed and converted to elemental sulphur.

The sweet gas is available for use as a fuel in the furnaces or in the hydrogen production plant burners.

1.5.7 Hydrogen production

In the hydrotreater, as previously explained, there is a big need for hydrogen.

The hydrogen requirements to produce refined petroleum products from bitumen are estimated to be 5-10 times larger than those used to produce the equivalent refined products from conventional crude [19].

In order to produce the hydrogen required from the hydrotreater there are always hydrogen production plants.

The most used and economical hydrogen production plant is the natural gas steam reforming (SR).

Currently, almost all the refineries are provided with this unit.

The scheme, the process, and the reaction of the SR will be better analyzed in the reference case modeling section.

As an alternative for the SR unit, hydrogen can be produced with a gasification process. This part will be analyzed in the gasifier model.

CHAPTER 2 : Energy Demand Assessment

In this chapter, the demand of the main 'energy streams' related to the entire process of production of SCO is calculated. In the first section, the demand and production of energy related to the SAGD process is analyzed. In the second section a model will be developed in order to calculate the main streams involved in the upgrading process.

The size selected for the plant is 150000 bbls/day. This capacity is associated to a big size SAGD plant. Actually there are just three plants that are around this size (Firebag, Christina Lake and Foster Creek).In the next years many plants are planning to expand to reach this capacity [1].Therefore, 150000 bbls/day seems to be the most representative and

interesting size to simulate.

2.1 SAGD DEMAND

In all of the SAGD plants there is a certain demand of energy streams. The main streams involved in the process are:

- Demand of high pressure steam by the wells
- Demand of electricity by the CPS and bottomhole pumps
- Production of gas from wells and VRU
- Production/demand of water
- Demand of diluent

The flowsheet scheme of SAGD energy demand is shown in Figure 14.

The first three streams are the most important and are the ones that largely affect the energy consumption of a SAGD plant. The calculation of these streams is simple and can be easily done with the knowledge of just one parameter for each stream (SOR, EOR, PGOR). These parameters relate the streams to the bitumen production (BIT_{prod}). The meaning of each parameter is explained and the factors that affect each of them are analyzed. Furthermore, values of SOR and EOR of the main SAGD operating plants are provided. The values of SOR and EOR are taken in ranges. Two different scenarios for the demand, respectively (i) high energy scenario (HES) and (ii) low energy scenario (LES) are calculated. The values were taken or calculated from the annual presentation that operators of in situ oil sands schemes are required to present to the Alberta energy regulator (AER) [21].

The last two streams don't have a big impact on the energy consumption. Nevertheless, it is important to consider them especially in certain situations as will be explained later on in Section 2.1.4.



Figure 14: Flowsheet Scheme of SAGD energy demand

2.1.1 High Pressure Steam

The steam required from the wells is without any doubt the most influential variable of the entire process. The key parameter to measure the amount of steam required from the process is the steam to oil ratio (SOR). The SOR is the volume of steam needed to produce a volume unit of bitumen. SAGD processes with a low value of SOR are less energy intensive, because of the big amount of energy related to the production of steam. On the other hand processes with high value of SOR results in a more expensive operation. The SOR can be cumulative (cSOR) or instantaneous (iSOR). The cSOR expresses the average volume of steam required to produce a unit volume of water over all the life of the project while the iSOR gives the instantaneous value in one specific moment. The cSOR and the iSOR can be used to evaluate the performances either of a well pair, a pad, a phase or an entire SAGD plant.

The SOR depends on many variables. The reservoir original properties combined with the operating parameters are the main variables affecting the SOR value. The reservoir properties involved are mainly porosity, initial pressure, initial temperature and initial saturation. The operational parameters are mainly pressure and temperature of the steam chambers that are dependent on the technology adopted for wells and artificial lift. Generally operation with low steam chambers pressures requires lower values of SOR. Because of that, as was mentioned earlier, ESPs are preferred to gas lift [22]. ESPs are usually operating in a range of pressure between 18-40 bar with a maximum temperature of 250°C [23].

A single well during its whole life have different phases related with different values of iSOR and cSOR. In the first few months the steam in injected to put in communication the two wells without any production (start-up).Since the well is not producing yet, the values of iSOR are enormous.

In the second phase (ramp-up) the wells start to produce and the iSOR starts to decrease (and consequently does the cSOR) until the steam chamber has reached its full vertical dimension. This phase lasts between 0.5 and 1.5 years.

When the chamber is fully grown the conventional SAGD phase starts. The value of iSOR are really low (between 2 and 2.5) and the cSOR starts to converge to the iSOR value. This phase lasts between 3 and 6 years.

After this starts the steam ramp-down when the amount of steam injected is sharply reduced while the production of bitumen is reduces gradually. This phase lasts less than 1.5 years and both the SORs continue to lower their value.

Then the steam stops to be injected and the chamber is maintained in pressure by injection of non-condensable gases while a small amount of bitumen is still produced (blowdown). The iSOR is zero while the cSOR continue to reduce [10]. The different phases of a well pair are shown in Figure 15.

Because of the high number of well pairs operating at the same time in one SAGD plant it is normal to refer to a unique value of cSOR and iSOR, which are representative of all the well pairs of the plant. This value is more steady than the ones referred to the pads or the phases but it is anyway variable during the lifetime of a SAGD plant. If a big expansion with new pads ramping up is done in a SAGD plant with most of the wells in a conventional phase , the values of the SORs increase. On the other hand if in one SAGD plant some new pads start up while others are in the ramp down, the value of the SORs of the plant won't change very much.

In Table 1 the values of SOR of some plants in Alberta are summarized. The steam injected in the wells should be produced in the steam generators at a pressure large enough to win the pressure drops in the pipes until the reservoir and to maintain the target pressure in the steam chamber.



Figure 15:Wellpair type curve from [13]

Typically the steam is produced at 70-110 bar and separated from the liquid water after the steam generation (usually OTSGs produce steam with 78-80% quality). A demand of pure saturated steam at 100bar and 311°C is considered. These values are typical for a SAGD extraction plant with ESPs like the one in [24]. The equation to calculate the Steam Demand for the extraction (SD_{ext}) is:

$$SD_{sat@100bar-ext} = BIT_{prod} * iSOR$$
 (2.1)

Since the demand of steam depends just on the value of iSOR and since this value is extremely changeable from one plant to another, a range of values for the iSOR is used. Most of the values of iSOR are contained into the range between 2 and 3 [21]. The actual iSOR values for Christina Lake and Firebag plants are considered related to a particular situation and will probably enter soon in that range. Because of that, a range of iSOR of 2-3 is taken.

Company	Plant	First Well Production ¹	Last Expansion	Nominal Size	cSOR ²	iSOR
Suncor	Firebag	2004	2012	190000	3.36	3.24
Suncor	MacKay River	2002	-	33000	2.4	2.6
CNRL	Kirby	2013	-	40000	5	NS
Cenovus	Foster Creek	2001	2009	120000	2.36	2.68
Cenovus	Christina Lake	2002	2013	140000	2	1.75
CNOOC Ltd.	Long Lake	2008	-	72000	4.5	NS
ConocoPhillips	Surmont	2007	-	30000	3.46	2.42
Devon	Jackfish 1	2007	-	35000	2.5	2.19
Devon	Jackfish 2	2011	-	35000	3	2.85
Husky	Tucker	2006	-	30000	5.83	NS

Table 1: cSOR and iSOR of the most important SAGD plant actually operative.

1 The First well Production year, Last Expansion and Nominal size (2013) are taken from **[1]**. 2 The values of cSOR and iSOR are taken from the 2014 presentations of the SAGD plant available from **[21]**

2.1.2 Electricity

In a SAGD plant there is a certain consumption of electricity. The electricity is demanded by all the electrical components of the SAGD plant.

The main component that are using electricity are the bottom hole pumps, the surface circulating pumps of the CPF, and the compressors of the vapor recovery unit. As was mentioned, the softening of water can be done with warm line softeners (WLS) or evaporators. The first option is the most used and, even if it produces water with more impurities, has a lower consumption of electricity. The higher consumption of electricity of evaporators is related to the presence of compressors.

In this study, the graphs of the electricity consumption of the main SAGD plants actually operating were related to the mean bitumen production for the examined period. The result is an index measured in kWh/bbl of bitumen. This index is calculated in order to make a parameter similar to the SOR and to predict easily the demand of electricity of a SAGD plant by the knowledge of the mean bitumen production. This index was called electricity to oil ratio (EOR). The results are shown in Table 2. The EOR is usually varying in a range between 8-15 KWh/bbl.

Company	Plant	Type of Softening	Gas sweetening	<i>BIT_{prod}</i> (bbl/day)	iSOR	EOR
Suncor	Firebag	WLS/EVA	Yes	147508	3.24	15.23
Suncor	MacKay River	WLS/EVA	No	25823.3	2.6	11.41
Cenovus	Foster Creek	WLS	Yes	109414	2.68	10.01
Cenovus	Christina Lake	WLS	Yes	143800	1.75	6.78
Conoco Phillips	Surmont	WLS	No	27135	2.42	8.37
Devon	Jackfish 1	WLS	Yes	35000	2.19	8.03
Devon	Jackfish 2	WLS	Yes	26000	2.85	8.95

Table 2: EOR of the main operative SAGD plant

All the data are taken from the 2014 presentations of the SAGD plant available from [21]. The Bitumen Production and the iSOR are related to one period. Every period considered is different depending on the data available

Generally the plant with a smaller iSOR has also a smaller value of EOR. The main reason for this is that both the bottom hole and the circulating pumps are working with a smaller flow rate of liquid and therefore consume less electricity. It is important to refer to the iSOR over the period of observation of the electricity consumption. In fact, the demand of electricity is not related to the history of the steam demand of the plant (cSOR), but just to its instantaneous value (iSOR).

SAGD plant with evaporators undergoes a bigger consumption of electricity. Some plants do not have a sweetening unit for production gas. The sweetening unit contributes to a higher demand of electricity because of the presence of additional electric components. It's important to say that just small plants can operate without a sweetening unit without exceeding the limits of SO2 emissions (Figure 9). All the large plants, if they want to use or flare the production gas, need to install a proper sweetening unit to meet the SO2 emissions requirements.

The equation to calculate the electricity demand for the extraction (ED_{ext}) is:

$$ED_{ext} = BIT_{prod} * EOR \tag{2.2}$$

Where *BIT*_{prod} is the production of bitumen (bbl/days).

The EOR changes a lot between one plant and another. Consequently, the electricity demand is variable for plants with the same size but different EOR. Because of that, a range of values will be taken for our analysis. The value of EOR for the LES (low energy scenario) is 7,5. This should correspond to a plant with SOR of 2 and just WLS. The value of EOR for the HES is 14. This should indicate a plant with SOR of 3 and installation of evaporators for ZLD.

2.1.3 Produced Gas

During the heavy oil bitumen recovery by SAGD there is a significant production of solution gas.

The emulsion coming from the wells contains some gas which is properly separated in the central process facility (CPS), desulphurized and used in the OTSGs.

The amount of solution gas from the wells is mainly quantified by the gas oil ratio (GOR) parameter, which measures the Sm3 gas dissolved in one Sm3 of bitumen.

The produced gas is mainly composed of CH_4 and CO_2 with a small amount of N_2 , H_2 heavier hydrocarbons and H_2S .

It is really important to predict the amount of solution gas from the wells and its composition in order to estimate successfully the heat power that it could produce in the OTSGs.

There have been a lot of attempts to estimate the amount of non-condensable gases dissolved in the produced liquids and the phenomenon of dissolution. According to these studies the main parameters involved in the process are the characteristics of the reservoir (permeability, original conditions and property of bitumen) and the operating conditions of the steam chamber (pressure and temperature).

The composition and the GOR can be really different from one area to another. In Athabasca, GOR value can vary from 2-6, although occasionally can have bigger values in some areas. Reasonable values for the composition can be [11]:

- 40-70 %mol C1
- 35-55 %mol CO₂
- 1-1.5 %mol H₂S
- 0.5-1.5 %mol N₂
- <1%mol H₂

The amount of heaver hydrocarbons is small and the methane to ethane ratio is usually high.

The values indicated by Canadian oil sands innovative alliance (COSIA) [25] for a typical produced gas are not far from Thimm's indications (Figure 16). The gas produced from the wells is not the only gas recovered in the SAGD process. There is some vapor that is recovered during the process from the VRU, mostly coming from FWKOs and tanks. These vapors are mainly composed of hydrocarbons (C1-C5+), CO₂ and H₂S.

The total Produced gas of the plant is the sum of the solution gas and the vapors recovered in the CPF. A typical composition is shown in Figure 16. The total amount of gas treated by the AGR cannot be quantified just by the GOR parameter. In fact, the GOR estimates only the non-condensable gases dissolved in the emulsion and does not consider the vapors from the dilbit.

Produced Gas Composition		Sour CP	F Produc	ced Gas
		Compos	ition (Dry	Basis)
H2	0.3 Mol%	H2	0.2	Mol%
CO2	30.0 Mol%	CO2	43.1	Mol%
N2	1.3 Mol%	N2	0.9	Mol%
H2S	0.13 Mol%	H2S	0.3	Mol%
C1	63.6 Mol%	C1	48.9	Mol%
C2	1.63 Mol%	C2	1.4	Mol%
C3	1.98 Mol%	C3	2.0	Mol%
C4	0.3 Mol%	C4	0.3	Mol%
C5+	0.88 Mol%	C5+	6.7	Mol%
(comp	at test separator)			

Figure 16: Typical values of Produced gas composition and Sour CPF Produced gas from [25]

In order to estimate the amount of produced gas from all the SAGD. This new parameter created was named produced gas to oil ratio (PGOR).

As can be determined from the COSIA typical process [25], a correct value for this parameter can be double the value of the GOR. Current values of the PGOR can be in a range between 4 and 12.

It is important to remember that the PGOR is quantifying the amount of sour gas before the AGR. After the AGR, the amount of sweet gas and its composition are different due to the removal of Sulphur (and some CO2). On the other hand its heating value is more or less the same before and after the sweetening.

The equation to calculate the sour produced gas for the extraction (SPG_{ext}) is:

$$SPG_{ext} = BIT_{prod} * PGOR$$
 (2.3)

Since this stream is much smaller than some other parameters involved in the SAGD process, it is taken just one value for the PGOR parameter. Accordingly to the COSIA typical process [25] a GOR of 5 and a PGOR of 10 are taken.

2.1.4 Water and Diluent

The three streams previously described can represent properly the energy streams demand and production of a SAGD plant. Nevertheless, energy is not the only important factor of a plant.

A proper use of water in a SAGD plant is very important. In Athabasca, water is not an abundant resource while all the processes involved are water intensive.

Generally speaking water can be produced or lost from the wells. The first case happens when the reservoir contains an aquifer. The mass of liquid water produced therefore is higher than the mass flow of steam water injected. On the other hand, if there is no presence of water in the reservoir, some losses of water should be considered. In that case, the mass of liquid water produced will be lower than the mass flow of steam water injected. The parameter that is measuring this phenomenon is called produced water to steam ratio (PWSR) and can be higher or lower than 1. Reasonable values of PWSR can be between 0.9 and 1.2.

Since the water coming from the wells is full of harnesses and impurities, a makeup and a disposal of water is always required and mandatory. Nevertheless, the

production/consumption of water from the wells can influence the plant design of the CPF. A situation where water is not produced from the wells requires a bigger make up than a situation where there is a PWSR bigger than one. If the location is particularly water deficient a solution with evaporators can be mandatory in order to use less water. On the other hand, if the reservoir is producing water there is no need to install evaporators and have a bigger demand of electricity.

Another stream that is involved in a SAGD plant is the Stream of Diluent.

As was mentioned in Section 1.5.1, it is mandatory to add diluent in order to transport the product in pipelines. The amount of diluent added and demanded from the SAGD plant is different from case to case depending on the quality of the bitumen. A typical composition of the dilbit can be around 30%vol of diluent and 70%vol of Bitumen. The diluent is then recovered during the upgrading and sent back to the CPF. A small part of diluent is always lost, and because of that a makeup of naphtha is always required.

Since the recovery rates are very high, the makeup of naphtha required is usually small. However, the makeup can be easily taken from the products of the upgrading (Section 2.2).

Nevertheless, if the refinery is very far from the SAGD there can be a significant increase of electricity consumption due to the transport of dilbit and diluent.

2.1.5 SAGD demand Result

In this section, the results for the demand of energy of a SAGD extraction plant is shown.

The input parameters of SOR, EOR and PGOR and their ranges are the one selected in the previous sections.

The results refer to a SAGD plant of $BIT_{prod} = 150000$ bbls/day. The results are shown in Table 3.

The amount of steam requested is enormous. Conversely, the amount of electricity requested is not very big. Every medium size gas turbine can provide that electricity without any problem. The produced gas flow rate is very small.

Parameter ID	Description	Units	LES ¹	HES ²
iSOR	instantaneous steam to oil ratio	Sm3 CWE/Sm3Bit	2,00	3,00
PGOR	produced gas to oil ratio	Sm3 gas/ Sm3 bit	10,00	10,00
EOR	electricity oil ratio	kWh/bbl bit	7,50	14,00
$ ho_{BIT}$	bitumen density	kg/m3	1003,00	1003,00
$ ho_{H2O}$	standard liquid water density	Kg/m3	999,54	999,54
$ ho_{SPG}$	density of sour produced gas	Kg/m2	1.31	1.31
BITprod	bitumen production	bbl/d	150000,00	150000,00
		kg/s	276,85	276,85
		Sm3/d	23848,10	23848,10
		MW	11813,09 ³	11813,09 ³
SPG _{ext}	sour produced gas from SAGD extraction	Sm3/d	238480,95	238480,95
		Sm3/s	2,76	2,76
		Kg/s	3,61	3,61
		MW	73,36 ¹	73,36 ¹
SD _{Sat@100bar-ext}	demand of high pressure saturated steam at 100 bar	m3/d CWE	47696,19	71544,29
		kg/s	551,79	827,68
		MW	1210,29 ¹	1815,43 ¹
ED _{ext}	electricity demand	MWh/year	410625,00	766500,00
		MWh/day	1125,00	2100,00
		MW	46,88	87,5

Table 3:	Energy	Demand	Streams	for	SAGD	extraction

1 LES refers to low energy scenario with iSOR=2 and EOR=7.5

2 HES refers to high energy scenario with iSOR=2 ans EOR=14

3 The Lower heating values and specific enthalpies parameters used for the conversion from flow rate and power are shown in Table 15.

2.2 UPGRADING DEMAND

In all units of the upgrading process there is a certain demand of energy streams. The main streams involved in the process are:

- Demand of heat/fuel in the furnaces
- Demand of MP Steam
- Demand of electricity
- Demand of hydrogen
- Production of fuel gas from the units
- Production of petcoke



Figure 17: Flowsheet scheme of upgrading process demand

The analysis of the energy demand from the utilities is not as simple as the one made for the SAGD extraction model. In order to predict the demand and production of energy streams, it is necessary to model and simulate the upgrading process. The general model consists of these units:

- Diluent recovery unit (DRU)
- Delayed coker (DC)
- 3 hydrotreaters (HTRs) for naphtha, light gas oil and heavy gas oil

The flow sheet scheme of the upgrading demand is shown in Figure 17. A model with the presence of a vacuum distillation unit was also considered, but was eliminated because was not bringing significant benefits.

The first step for the prediction of the energy demand is the calculation of all the streams involved in the processes. In order to do that, many equations available in the literature were used to model the units [26] [27]. Then, other correlations to calculate the demand of energy flows were used [20]. These correlations link the demand of energy vectors to some of the streams previously calculated.

2.2.1 Calculation of the main streams involved

In this section, the main streams involved in the process are calculated.

For the streams described, this notation is used:

STREAM_{feed}/prod-UNIT

Where the possible streams and their acronyms are:

DB = diluted bitumen BIT = bitumen ATB = atmospheric topped bitumen NPH = naphtha LGO = light gas oil HGO = heavy gas oil PCK = petroleum coke FG = fuel gas

While the acronyms for the units are:

DRU = diluent recovery unit DC = delayed coking NPH HTR = naphtha hydrotreater LGO HTR = light Gas oil hydrotreater HGO HTR = heavy gas oil hydrotreater

At the end of each group of equations introduced, a table will be provided with the description of the parameters involved in the equations and their values. In Table 8 then, the results of the main streams involved are illustrated.

Diluent Recovery Unit:

The streams involved in the DRU are:

$$DB_{feed-DRU} = BIT_{prod} * (1 + DR)$$
(2.4)

$$LGO_{prod-DRU} = DB_{feed-DRU} * YLD_{LGO-DRU}$$
(2.5)

$$NPH_{prod-DRU} = BIT_{prod} * DR * RF_{NPH-DRU}$$
(2.6)

$$NPH_{MakeUp} = BIT_{prod} * DR * (1 - RF_{NPH})$$
(2.7)

$$ATB_{prod-DRU} = DB_{feed-DRU} - LGO_{prod-DRU} - NPH_{prod-DRU}$$
(2.8)

The values and the descriptions of the parameters mentioned above are shown in Table 4. Theparameters used for the DRU are actually experimental data of the DRU of Syncrude upgrading plant that have been published in [28].

Parameter-ID	Description	Units	Value
DR	Diluent requirements of SAGD bitumen	KgDIL/kgBIT	0,23
RF _{NPH-DRU}	Recovery factor of naphtha in DRU	% of feed	0,98
YLD _{LGO-DRU}	LGO yield in DRU	% of feed	0,14
API _{lgo-dru}	API Gravity LGO	API	25,99

Table 4: Parameters of DRU

Delayed coker:

The equation used to calculate the products and yields of the delayed coker are based on three parameter [26]:

• Conradson carbon ratio (*CCR_{ATB}*)

- Sulphur yield of the feed $(YLD_{SULPHUR-ATB})$
- Specific Gravity (*SG*_{ATB})

These values are referred to the ATB_{prod} produced by the DRU and entering the coker. The equation used to calculate the yields, the densities and the sulphur contents of the products were taken from HPI [26]:

$$YL_{RG-DC} = 3.5 + 0.01 * CCR_{ATB}$$
(2.9)

$$YLD_{C3-C4-DC} = 4.3 + 0.044 * CCR_{ATB}$$
(2.10)

$$YLD_{NPH-DC} = 11.38 + 0.335 * CCR_{ATB}$$
(2.11)

$$YLD_{PCK-DC} = 1.6 * CCR_{ATB}$$

$$(2.12)$$

$$YLD_{Gasoil-DC} = 100 - YLD_{RG-DC} - YLD_{C3-C4-DC} - YLD_{NPH-DC} - YLD_{PCK-DC}$$
(2.13)

$$\frac{LGO}{Gasoil_{RATIO}} = 0.38 + 0.011 * CCR_{ATB} - 0.0003 * CCR_{ATB}^{2}$$
(2.14)

$$YLD_{LGO-DC} = YLD_{Gasoil-DC} * \frac{LGO}{Gasoil_{RATIO}}$$
(2.15)

$$YLD_{HGO-DC} = YLD_{Gasoil-DC} - YLD_{LGO-DC}$$

$$(2.16)$$

$$API_{NPH} = 55 \tag{2.17}$$

$$API_{LGO} = 36 \tag{2.18}$$

$$API_{HGO} = \frac{141.5}{0.528 * SG_{ATB} + 0.4053} - 131.5$$
(2.19)

$$YLD_{S-NPH} = 0.14 * YLD_{S-ATB}$$

$$(2.20)$$

$$YLD_{S-LGO} = 0.45 * YLD_{S-ATB} \tag{2.21}$$

$$YLD_{S-HGO} = 0.82 * YLD_{S-ATB}$$

$$(2.22)$$

The equations receives as an input the three parameters (CCR_{ATB} , SG_{ATB} , YLD_{S-ATB}) taken from [28]. The results are shown in Table 5.

According to Gary [20], the values calculated from these equations are accurate enough for primary economic study. The actual yields can be determined just by the pilot plant operation.

Table 5: Yields, Density and Sulfur content of the products of the Delayed Coker

Parameter-ID	Description		Value
CCR _{ATB}	Feed Conradson carbon residue of ATB		13,5
API _{ATB}	API gravity ATB	API	6,7
SG_{ATB}	Specific gravity ATB		1,024

YLD _{S-ATB}	Feed sulfur content of ATB	%wt	4,78
YLD_{RG-DC}	refinery gas yield in delayed coker	%wt	4,85
$YLD_{C3-C4-DC}$	LPG yield in delayed coker	%wt	4,894
YLD_{FG-DC}	fuel gas yield in delayed coker	%wt	9,744
YLD _{NPH-DC}	naphtha yield in delayed coker	%wt	15,90
YLD _{PCK-DC}	coke yield in delayed coker	%wt	21,6
YLD _{Gasoil-DC}	total gasoil yield in delayed coker	%wt	52,75
LGO Gasoil _{RATIO}	weight ratio (LGO over total gasoil)	%	0,47
YLD_{LGO-DC}	LGO yield in delayed coker	%wt	25,00
YLD _{HGO-DC}	HGO yield in delayed coker	%wt	27,76
API _{NPH-DC}	API gravity naphtha delayed coker	API	55,00
API _{LGO-DC}	API Gravity LGO delayed coker	API	36,00
API _{HGO-DC}	API gravity HGO delayed coker	API	18,09
YLD _{S-NPH}	naphtha product sulfur content	%wt	0,67
YLD_{S-LGO}	LGO product sulfur content	%wt	2,15
YLD _{S-HGO}	HGO product sulfur content	%wt	3,92

Once these values are calculated it is possible to calculate the main stream:

$$FG_{prod-DC} = ATB_{feed-DC} * YLD_{FG-DC}$$
(2.23)

$$NPH_{Prod-DC} = ATB_{feed-DC} * YLD_{NPH-DC}$$
(2.24)

$$LGO_{Prod-DC} = ATB_{feed-DC} * YLD_{LGO-DC}$$
(2.25)

$$HGO_{Prod-DC} = ATB_{feed-DC} * YLD_{HGO-DC}$$
(2.26)

$$PCK_{Prod} = ATB_{feed-DC} * YLD_{PCK-DC}$$
(2.27)

Hydrotreating:

In our scheme three Hydrotreaters are in operation. Each one has a different feed:

$$NPH_{feed-NPH HTR} = NPH_{Prod-DC}$$
(2.28)

$$LGO_{feed-LGO HTR} = LGO_{prod-DRU} + LGO_{Prod-DC}$$
(2.29)

$$HGO_{feed-HGO \, HTR} = HGO_{Prod-DC} \tag{2.30}$$

The density and the sulphur contents of the feeds are shown in Table 6. Since the LGO produced in the DC has different values of density ($\rho_{prod-DC}$) than the LGO produced in the DRU ($\rho_{prod-DRU}$), the density of the mixture of the two streams ($\rho_{feed-LGOHTR}$) has to be calculated:

$$\rho_{feed-LGO \ HTR} = \frac{1}{\frac{LGO_{prod-DRU}}{LGO_{feed-HTR} + \frac{1}{\rho_{prod-DRU}} + \frac{LGO_{prod-DC}}{LGO_{feed-HTR} + \frac{1}{\rho_{prod-DC}}}}$$
(2.31)

$$API_{feed-LGO\ HTR} = \frac{141.5}{0.528*\frac{\rho_{feed}-LGO\ HTR}{\rho_{H2O}} + 0.4053} - 131.5$$
(2.32)

Where $\rho_{H20} = 999,12 \ kg/m3$ is the density of water in standard conditions.

Regarding the sulfur content, the values of the delayed coker product were assumed for the LGO hydrotreater. This assumption is not affecting the results.

The density and the sulphur content of the feed are important in order to calculate the hydrogen requirements (HR) of the HTRs. The HR of the three HTRs are probably ones of the most difficult parameters to calculate. The value of these parameters depend not just on the sulphur content but also on many other variables such as nitrogen content and olefin and aromatics specifications in the product.

The hydrogen consumption is therefore related to the desired specifications of the SCO and can vary a lot from case to case.



Figure 18 : Hydrogen request Vs sulphur % in feed (naphtha)



Figure 19: API increase Vs hydrogen input (naphtha)



Figure 20: Hydrogen request Vs sulphur % in feed (heavier fractions)



Figure 21:API increase Vs hydrogen input (heavier fractions)

Unfortunately there are no mathematical correlations used to predict the HR of the HTRs. Maples [27] has collected a large number of experimental data that were represented in two types of graphs that were used for the calculations.

The first graph represents the hydrogen required as a function of the sulphur feed percentage. The second one relates the hydrogen inlet to the increase in API gravity of the product. The graphs are available for naphtha (Figure 18 and 19) and heavier fractions feeds (Figure 20 and 21).

The graphs are be used in this way:

The Sulphur yield is entered into the first graph to get the hydrogen required to remove all the sulfur. This value is entered into the second graph in order to take the API gravity increase. This operation is repeated for all the HTRs feed. The SCO product has to meet some minimum specifications. If the final product meets these specification, the methodology used prove to be adequate, as it will be explained. The results of this process are shown into Table 7.

Parameter-ID	Description	Units	Value
YLD_{S-NPH}	Naphtha sulfur content	%wt	0,67
YLD_{S-LGO}	LGO sulfur content	%wt	2,15
YLD _{S-HGO}	HGO sulfur content	%wt	3,92
HR _{NPH HTR}	H ₂ required in hydrotreatment - naphtha	SCF/bbl	100

Table 6: Main parameters for the HTRs

		feed	
HR _{LGO HTR}	H ₂ required in hydrotreatment - LGO	SCF/bbl feed	620
HR _{hgo htr}	H ₂ required in hydrotreatment - LGO	SCF/bbl	805
API _{feed-NPH HTR}	density naphtha feed	API	55
API _{feed-LGO HTR}	density LGO feed	API	31,78
API _{feed-HGO HTR}	density HGO feed	API	18,09
API _{Prod-NPH HTR}	density naphtha product	API	55,2
API _{Prod-LGO HTR}	density LGO product	API	35,78
API _{Prod-HGO HTR}	density HGO product	API	24
YLD _{H2S-NPH HTR}	H ₂ S yield in naphtha ht	%wt	0.71
YLD _{FG-NPH HTR}	offgas yield in naphtha ht	%wt	0.69
YLD _{H2S-LGO HTR}	H ₂ S yield in LGO ht	%wt	2.17
YLD _{H2S-HGO HTR}	H ₂ S yield in HGO ht	%wt	3.75
YLD _{NPH-NPH HTR}	liquid yield in naphtha ht	%wt	98.6
YLD _{LGO-LGO HTR}	liquid yield in LGO ht	%wt	97.83
YLD _{HGO-HGO HTR}	liquid yield in HGO ht	%wt	96.25

The Hydrogen Demand (HD) is therefore:

$HD_{NPH \ HTR} =$	$NPH_{feed-NPH HTR} * HR_{NPH HTR}$	(2.3	3))
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$HD_{LGO \ HTR} = LGO_{feed-LGO \ HTR} * HR_{LGO \ HTR}$	(2.34)
--	--------

```
HD_{HGO \ HTR} = HGO_{feed - HGO \ HTR} * HR_{HGO \ HTR} (2.35)
```

In order to calculate the products streams, the conversion yields in the hydrotreater should be estimated.

According to Maples [27], when a large increase in API is reported for a stock, there is significant conversion of some of the feed into lower boiling materials.

In our case, for instance, the HGO's API has a significant increment, which means that part of the feed has been converted into LGO (and a small part into naphtha). These lower boiling materials are already included into the product. Because of that, a unique value for the liquid yield is taken for each hydrotreater.

In order to calculate the liquid yield, the gas yields have to be determined. In this regard, the correlations of HPI are used [26]:

 $YLD_{H2S-NPH HTR} = 1.063 * YLD_{S-NPH}$ (2.36)

$$YLD_{FG-NPH \ HTR} = 0.25 + 0.66 * YLD_{S-NPH}$$

$$YLD_{H2S-LGO \ HTR} = 1.01 * YLD_{S-LGO}$$
(2.37)
(2.38)
(2.38)

 $YLD_{H2S-HGO HTR} = 0.957 * YLD_{S-HGO}$ (2.39)

The yield of refinery gases from the gasoil HTRs was so small that can be neglected. The NH3 off gas was not considered because his flowrate is small and his analysis is not part of this work. The results are shown in Table 6.

The liquid yields are:

$$YLD_{NPH-NPH HTR} = 1 - YLD_{H2S-NPH HTR} - YLD_{FG-NPH HTR}$$
(2.40)

$$YLD_{LGO-LGO HTR} = 1 - YLD_{H2S-LGO HTR}$$

$$(2.41)$$

$$YLD_{HGO-HGO \ HTR} = 1 - YLD_{H2S-HGO \ HTR}$$
(2.42)

The product streams are:

$$NPH_{prod-NPH HTR} = NPH_{feed-NPH HTR} * (1 + HD_{NPH HTR}) * YLD_{NPH NPHHTR}$$
(2.43)

$$FG_{prod-NPH HTR} = NPH_{feed-NPH HTR} * YLD_{FG-NPH HTR}$$
(2.44)

$$LGO_{prod-LGO HTR} = LGO_{feed-LGO HTR} * (1 + HD_{LGO HTR}) * YLD_{LGO-LGO HTR}$$
(2.45)

$$HGO_{prod-HGO HTR} = HGO_{feed-HGO HTR} * (1 + HD_{HGO HTR}) * YLD_{HGO-HGO HTR}$$
(2.46)

$$H2S_{prod-HTRs} = NPH_{feed-NPH HTR} * (1 + HD_{NPH HTR}) * YLD_{H2S-NPH HTR} + LGO_{feed-LGO HTR} * (1 + HD_{LGO HTR}) * YLD_{H2S-LGO HTR} + HGO_{feed-HGO HTR} * (1 + HD_{HGO HTR}) * YLD_{H2S-HGO HTR}$$

(2.47)

Product SCO

The resulted upgraded SCO stream is:

 $SCO_{Prod} = NPH_{prod-NPH HTR} + LGO_{prod-LGO HTR} + HGO_{prod-HGO HTR} - NPH_{MakeUp}$ (2.48)The characteristics of the product are resumed in Table 7.

Parameter-ID	Description	Units	Value
YLD _{NPH-SCO}	Naphtha yield in SCO	% wt	0,18

Table 7: Characteristic of The SCO product

YLD _{LGO-SCO}	LGO yield in SCO	% wt	0,50
YLD _{HGO-SCO}	HGO yield in SCO	% wt	0,32
	Total	%	1,00
API _{SCO}	API density of SCO	API	35,64

The SCO should achieve some characteristics with the upgrading process. The main goal of the upgrading to SCO is the production of a product with similar characteristic of a light crude oil. Otherwise, the refineries won't be interested in buying a product very complicated to refine with their equipment.

The target set for the upgrading process was to produce a SCO with an almost complete removal of Sulphur and an API grade higher than 31.1 °API (lower limit for a light oil). The API gravity calculated has a value much higher than the minimum limit set (Table 7). This basically means that the product has a high standard quality and will be very competitive on the market.

The main streams involved in the upgrading process are then shown in Table 8.

Parameter-ID	Description	Units	Value
BIT _{prod}	bitumen production	bbl/d	150000,00
		bbl/h	6250,00
		kg/s	276,85
DB _{feed-DRU}	dilbit feed of DRU	kg/s	339,91
		bbl/h	8134,05
$LGO_{prod-DRU}$	LGO product from DRU	bbl/h	1098,10
		kg/s	43,55
NPH _{recov}	naphtha recovered	kg/s	61,80
NPH _{MakeUp}	naphtha makeup	kg/s	1,26
ATB _{prod-DRU}	ATB produced in DRU	kg/s	234,56
TOTAL _{prod-DRU}	total product of DRU	Kg/s	339,91
ATB _{feed-DC}	atmospheric topped bitumen feed of DC	kg/s	234,56
		bbl/h	5192,47
NPH _{Prod-DC}	Naphtha produced in DC	kg/s	37,30
LGO _{Prod-DC}	LGO produced in DC	kg/s	58,63
HGO _{Prod-DC}	HGO produced in DC	kg/s	65,11

 Table 8: Main streams involved in the upgrading process

$PCK_{Prod-DC}$	petcoke produced in DC	kg/s	50,66
FG _{prod-DC}	sour fuel gas produced in DC	kg/s	22,86
$TOTAL_{prod-DC}$	total product of DC	Kg/s	234,56
NPH _{feed-NPH HTR}	naphtha hydrotreater feed	kg/s	37,30
LGO _{feed-LGO HTR}	LGO hydrotreater feed	kg/s	102,18
HGO _{feed-HGO HTR}	HGO hydrotreater feed	kg/s	65,11
HD _{NPH HTR}	hydrogen demand naphtha hydrotreater	kg/s	0,08
HD _{LGO HTR}	Hydrogen demand LGO Hydrotreater	kg/s	1,34
HD _{hgo htr}	Hydrogen Demand HGO Hydrotreater	kg/s	1,24
HD _{UPGR}	Total Hydrogen Demand	kg/s	2,65
$TOTAL_{feed-HTRs}$	Total HTRs feed	kg/s	207,24
		bbl/h	5229,71
NPH _{prod-NPH HTR}	Naphtha Hydrotreater product	kg/s	36,86
LGO _{prod-LGO HTR}	LGO Hydrotreater product	kg/s	101,27
HGO _{prod-HGO HTR}	HGO Hydrotreater product	kg/s	63,86
H2S _{prod-HTRs}	H2S produced	kg/s	5,00
FG _{prod-NPH HTR}	Off-gas	kg/s	0,26
TOTAL _{prod-HTRs}	Total HTRs product	kg/s	207,24
NPH _{MakeUp}	Make up naphtha	kg/s	1,26
SCO _{Prod}	Synthetic Crude Oil Produced	kg/s	200,72

2.2.2 Heat/Fuel Demand

In the upgrading process there is a certain demand of heat/fuel from the different units. This fuel is used in furnaces to heat the feed to the operating temperature, in order to make the desired reactions.

The fuel requirements (FR) of every unit are taken from Gary [20] and shown in Table 9. According to Gary [20], the FRs already take into account the heater efficiency. In the upgrading plants, the fuel gas adopted in the furnaces is usually the sweet offgas from the units or natural gas. The fuel demand (FD) of the upgrading process is described by these equations:

$$FD_{DRU} = DB_{feed-DRU} * FR_{DRU}$$
(2.49)

$$FD_{DC} = ATB_{feed-DC} * FR_{DC}$$
(2.50)

$FD_{HTRS} = TOTAL_{feed-HTRS} * FR_{HTR}$	(2.	51)

 $FD_{UPGR} = FD_{DRU} + FD_{DC} + FD_{HTR}$ (2.52)

The equations show that the demand of heat/fuel is proportional to the feed flow rate.

Parameter-ID	Description	Units	Value
FR _{DRU}	Fuel requirements - DRU	MJ/bblfeed	52,75
FR_{DC}	Fuel requirements - DC	MJ/bblfeed	147,00
FR _{HTR}	Fuel requirements - HTR	MJ/bblfeed	211,00

 Table 9: Fuel Requirements of the Units from (13)

2.2.3 Steam Demand

All the units of the upgrading process have a certain steam demand.

The characteristic of the steam demanded are different from unit to unit. The DC requires high pressure superheated steam. This request of steam is in order to avoid the coke deposition into the furnace. The steam shouldn't cool down the feed into the furnace. Consequently. its temperature should be at least the same as that of the furnace temperature. Since the operational range temperature of DC is 480-515 °C, a temperature of 500°C and a pressure of 38.5 bar for the steam were selected.

The DRU and the HTRs require steam mainly for stripping. This steam should be saturated. Accordingly to Gary [20], saturated steam at 20 bar was selected. Differently from the steam of the DC, this stream comes out after stripping as a saturated liquid, and just needs the heat of evaporation to be provided.

The steam demands (SD) of the upgrading process are described by the following equations as a function of the Steam requirements (SR) of the units. The SR of the units are taken from Gary [20] and shown in Table 10.

$SD_{Sat@20bar-DRU} = DB$	$S_{feed-DRU} * SR_{DRU}$	(2.53)
Sucezobul Dro		

$SD_{@38.5bar,500^{\circ}C-DC} =$	$PCK_{Prod-DC} * SR_{DC}$	(2.54)
-----------------------------------	---------------------------	--------

$$SD_{sat@20bar-HTRs} = TOTAL_{feed-HTRs} * SR_{HTRs}$$
 (2.55)

$$SD_{@38.5bar,500^{\circ}C-UPGR} = SD_{@38.5bar,500^{\circ}C-DC}$$
(2.56)

$$SD_{Sat@20bar-UPGR} = SATSD_{Sat@20bar-DRU} + SATSD_{Sat@20bar-HTRs}$$
(2.57)

The steam demand is generally proportional to the feed flow rate. The DC demand instead, is proportional to the Petcoke production.

Parameter-ID	Description	Units	Value
SR _{DRU}	Steam consumption - DRU	kg/bblfeed	4,50
SR _{DC}	Steam consumption - DC	kg/tcoke	318,00
SR _{HTRs}	Steam consumption - HTR	kg/bblfeed	4,50

Table 10: Steam Requirements from (13)

2.2.4 Electricity Demand

All of the units of the upgrading process have a consumption of electricity.

The electricity is mainly used to pump the fluids into the units by circulating pumps. In the DC electricity requirements (FP) include the motor drive electricity consumption.

In the DC, electricity requirements (ER_{DC}) include the motor drive electricity consumption for the hydraulic decoking pump.

The HTRs are by far the units with the highest consumption of electricity, due to the presence of compressors for the hydrogen.

The electricity demand (ED) of the upgrading process is calculated from the electricity requirements of every unit, shown in Table 11 and taken from Gary [20]. These are the equations that describes the ED:

$$ED_{DRU} = DB_{feed-DRU} * ER_{DRU}$$
(2.58)

$$ED_{DC} = PCK_{Prod-DC} * ER_{DC}$$
(2.59)

$$ED_{HTRs} = TOTAL_{feed-HTRs} * ER_{HTRs}$$
(2.60)

$$ED_{GO} = (ED_{DRU} + ED_{DC} + ED_{HTRs}) * ER_{GO}$$

$$(2.61)$$

$$ED_{UPGR} = ED_{DRU} + ED_{DC} + ED_{HTRs} + ED_{GO}$$
(2.62)

The electricity demand is generally proportional to the feed flow rate. The DC demand instead, is proportional to the petcoke production.

Parameter-ID	Description	Units	Value
ER_{DRU}	Electricity requirements -DRU	kWh/bblfeed	0,90
ER_{DC}	Electricity requirements - DC	kWh/tcoke	30,00
ER _{HTRs}	Electricity requirements - HTR	Kwh/bblfeed	6,00
ER _{GO}	Electriciy for general Operations	%	0,10

 Table 11: Electricity requirements from (13)

2.2.5 Hydrogen demand

In the upgrading process of bitumen there is a large demand of hydrogen. The hydrogen request (HR) and demand (HD) for every HTR were already calculated in Section 2.2.1. The total hydrogen demand for the upgrading process is the sum of the demand of every unit.

The HR parameters calculated previously are reported again in Table 12.

$$HD_{UPGR} = HD_{NPH \ HTR} + HD_{LGO \ HTR} + HD_{HGO \ HTR}$$
(2.63)

Parameter-ID	Description	Units	Value
HR _{NPH HTR}	H ₂ required in NPH HTR	SCF/bbl feed	100
HR _{lgo htr}	H ₂ required in LGO HTR	SCF/bbl feed	620
HR _{hgo htr}	H ₂ required in HGO HTR	SCF/bbl	805

Table 12: Hydrogen requirements of HTRs

2.2.6 Fuel gas production

In the upgrading of bitumen to SCO, there is a certain production of fuel gas. This gas contains the lighter hydrocarbons of the bitumen (C1-C4) and can be used as a fuel in the furnaces, in the natural gas steam reformer or in steam generations. The fuel gas is produced mainly in the DC and in the HTRs. The equations for the fuel gas production (FG_{prod}) are:

$r \approx proa - DC$ $r = DC$ $r = DC$ $r = DC$ $(=, 0)$	$TB_{feed-DC} * YLD_{FG-DC} \tag{2.64}$
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```
FG_{prod-NAPHTHA\,HTR} = NPH_{feed-NPH\,HTR} * YLD_{C1-C4-NPH\,HTR} (2.65)
```

$$FG_{prod-UPGR} = FG_{DC} + FG_{prod-NPH HTR}$$
(2.66)

Since the offgas produced in the naphtha HTRs is almost two orders of magnitude lower than the offgas in the DC, the composition of the total offgas is considered equivalent to the one of the DC. The gas composition considered is provided by HPI [26] and shown in Table 13.

Parameter-ID	Name	Yield (%wt)	
H2	Hydrogen	0.8	
C1	Methane	26.7	

Table 13: Composition of the offgas produced in the upgrading

C2-	Ethylene	3.0
C2	Ethane	18.7
С3-	Propylene	8.3
C3	Propane	17.9
C4-	Butenes	10.1
iC4	Isobutane	3.8
nC4	N-butane	9.5
H_2S	Hydrogen sulfide	1.2

2.2.7 upgrading demand results

In this Section the results for the demand of energy vectors of the upgrading process are shown in Table 14.

Parameter-ID	Description	Units	Value
BIT _{prod}	Bitumen input	bbl/d	150000,00
		bbl/h	6250,00
		kg/s	276,85
		MW	11813,09
SCO _{Prod}	SCO produced	kg/s	133035,53
		bbl/h	5543,15
		bbl/d	207,24
		MW	9645,08
<i>HD_{UPGR}</i>	Hydrogen demand upgrading	kg/s	2,65
		MW	318,42 ¹
PCK _{Prod-DC}	Petcoke produced	kg/s	50,66
$FG_{prod-DC}$	Sour fuel gas produced in DC	kg/s	22,86
FG _{prod-NPH HTR}	Sour fuel gas produced in Naphtha HTRs	kg/s	0,26
$FG_{prod-UPGR}$	Fuel gas produced in Upgrading	kg/s	23,11
		MW	1098.84
FD_{DRU}	Fuel demand DRU	MW	119,19
FD _{DC}	Fuel demand for DC	MW	212,03

Table 14: Results of upgrading demand

FD _{HTRs}	Fuel Demand HTR	MW	306,52
FD _{UPGR}	Total fuel demand	MW	637,73
SD _{Sat@20bar-DRU}	Steam demand DRU	kg/s	10,17
SD _{@38.5bar,500°C-DC}	Steam demand DC	kg/s	16,11
SD _{Sat@20bar-HTRs}	Steam demand HTR	kg/s	6,54
SD _{@38.5bar,500°C-UPGR}	Superheated steam	kg/s	16,11
		MW	55,42
SD _{Sat@20bar-UPGR}	Saturated Steam	kg/s	16,70
		MW	32,74
ED _{DRU}	Electricity demand - DRU	Mwh/year	64128,82
ED _{DC}	Electricity demand in the DC	Mwh/year	47933,14
ED _{HTRs}	Electricity demand in the HTR	Mwh/year	274873,60
ED_{GO}	Electricity demand for plant operations	Mwh/year	38693,56
ED _{UPGR}	Total electricity demand for the upgrading	Mwh/year	425629,11
		MW	48,59

1 The Lower Heating values and specific enthalpies parameters used for the conversion from flow rate and power are shown in Table 15.

Parameter-ID	Description		Value
LHV_{SPG}^{1}	lower heating value of sour produced gas	MJ/kg	20,33
LHV_{H2}^{1}	lower heating value of hydrogen	MJ/kg	119,96
LHV_{FG}^{1}	lower heating value of sour fuel gas from upgrading		47,54
LHV_{BIT}^{2}	lower heating value of bitumen		42,67
LHV _{SC0} ²	lower heating value of synthetic crude oil	MJ/kg	46,54
$\Delta h_{Sat@100bar}^{3}$	variation of specific enthalpy between the inlet ¹ and outlet condition of high pressure saturated steam	MJ/kg	2,19
$\Delta h_{@38.5bar,500} \circ c^3$	variation of specific enthalpy between the inlet and outlet condition of superheated steam at 38.5 bar and 500°c	MJ/kg	3,44
$\Delta h_{Sat@20bar}^{3}$	variation of specific enthalpy between the inlet and outlet condition of saturated steam at 20 bar	MJ/kg	1,96

Table 15:	LHVs and	differences	of enthal	pies of tl	he main	streams	involved

1 The LHV of these streams have been calculated with the software Aspen Plus [29] with as an input the composition of the streams and their thermodynamic conditions

2 Values from National Energy Board website as mean values for Athabasca bitumen and SCO [30]

3 The inlet conditions for every stream are the one used in Chapter 3 for the energy facilities.

2.3 TOTAL DEMAND

In order to build the energy infrastructure, the total requirements of the processes have to be calculated. These requirements are the sum of the demands of the SAGD extraction process and of the upgrading to SCO.

The steam required by the extraction has different characteristics from the steam demanded by the upgrading. Likewise, the produced gas from the wells has different characteristics and use than the off gas produced from the upgrading process.

The only streams that can be actually added are the demands of electricity. Here are the main calculation for the total demand:

$SCO_{Prod} = SCO_{Prod-UPGR}$	(2.67)
$SPG_{tot} = SPG_{extr}$	(2.68)
$FG_{prod-tot} = FG_{prod-UPGR}$	(2.69)
$PCK_{Prod-tot} = PCK_{Prod-UPGR}$	(2.70)
$SD_{Sat@100bar} = SD_{Sat@100bar-ext}$	(2.71)
$SD_{@38.5bar,500^{\circ}C} = SD_{@38.5bar,500^{\circ}C-ext}$	(2.72)
$SD_{Sat@20bar} = SD_{Sat@20bar-ext}$	(2.73)
$FD_{tot} = FD_{UPGR}$	(2.74)
$HD_{tot} = HD_{UPGR}$	(2.75)
$ED_{tot} = ED_{ext} + ED_{UPGR}$	(2.76)

The results of these equations are shown in Table 16.

The flowsheet of the total demand of energy streams associated to the process is shown in Figure 22.

Table 16: Total result of Energy stream demand related to extraction and upgradingto SCO

Parameter ID	Description	Units	LES ¹	HES ²
BIT _{prod}	bitumen production	bbl/d	150000,00	150000,00
		kg/s	276,85	276,85
		MW	11813,09	11813,09
SCO _{Prod}	SCO produced	Bbl/d	133035,53	133035,53
		kg/s	207,24	207,24
		MW	9645,08	9645,08
SPG _{tot}	total sour produced gas	Kg/s	3,61	3,61

		MW	73,37	73,37
FG _{prod-tot}	fuel gas produced	kg/s	23,11	23,11
		MW	1098.84	1098.84
PCK _{Prod-tot}	petcoke produced	kg/s	50,66	50,66
SD _{Sat@100bar}	demand of high pressure saturated steam at 100 bar	kg/s	551,79	827,68
		MW	1210,29	1815,43
SD _{@38.5bar,500°C}	demand of superheated steam at 38.5bar and 500°c	kg/s	16,11	16,11
		MW	55,42	55,42
SD _{Sat@20bar}	demand of saturated steam at 20bar	kg/s	16,70	16,70
		MW	32,74	32,74
FD _{tot}	fuel demand for upgrading	MW	637,73	637,73
<i>HD_{tot}</i>	total hydrogen consumption	kg/s	2,65	2,65
		MW	318,42 ¹	318,42
ED _{tot}	electricity demand per year	MWh/yr	836254,11	1192129,11
		MW	95,46	136,09
ST/PWR	Steam/power Ratio	MW _{steam} /MW _{power}	13.6	13.99

1 LES refers to low energy scenario with iSOR=2 and EOR=7.5

2 HES refers to high energy scenario with iSOR=2 ans EOR=14 $\,$



Figure 22: Flowsheet of the total demand of the process

CHAPTER 3: Reference Case Model

In the previous chapter the total demand of energy streams related to the entire SAGD extraction and upgrading process has been calculated.

In this chapter a reference case (RC) model will be generated in order to satisfy the demand of all the energy streams previously calculated.

Furthermore, this model will calculate the fuel consumption of the energy facilities and the related CO2 emissions. The model will be provided and simulated with the software Aspen Plus from Aspentech [29].

In the reference case the main fuel used to satisfy the demand of energy vectors is natural gas from the pipeline. The average composition of western Canadian natural gas is taken from Uniongas website [31] and shown in Table 18.

3.1 STRUCTURE OF THE ENERGY FACILITIES

The structure of the energy facilities has been selected from the experience and the knowledge of the real facilities operating in the bitumen extraction and upgrading processes. The study of the major operative plants has been taken from the performance presentation available from the AER [21].

Regarding the commercial energy facilities used by the companies, some observations can be made:

- Some plants are buying electricity from the grid while others are producing their own electricity.
- The plants that have gas turbines usually have OT-HRSG for cogeneration [21].
- It is possible to export electricity to the grid, although there are some limits (usually less than 100 MW due to the limit of the current electric grid)
- In SAGD plants, companies prefer to modularize and use small-medium size gas turbines. In operating plants, it is difficult to find a unit bigger than 70-80 MWe. The main reason is that Alberta's severe climate conditions create problems in transport, installation and maintenance of large size units.
- Due to the use of warm lime softeners for softening, the use of OTSGs is mandatory. Nevertheless, some plants are using evaporators on the blowdown of the OTSGs in order to maximize the water recycling.
- The fuel used by the OTSGs is mainly natural gas bought from the pipeline. The produced gas can be used in the plant after sweetening as co-fuel in OTSGs. No plants are burning solid/liquid fuels in OTSGs.
- The SAGD extraction and upgrading plants are usually separated by several kilometers. That makes the transport of gaseous fluids impossible (as the offgas from the upgrading) from one area to another. Electricity can be transported without any problem.

- The main technology used for hydrogen production is the natural gas steam reforming in tubular furnaces. This technology co-produces steam.
- The supplementary steam requirements of the upgrading can be generated with drum Boilers or with cogenerative steam cycles.
- The direct combustion of petcoke is possible but strongly discouraged because of its sulphur content. There are severe limits to sulphur emissions.
- The gas generated in the upgrading area can be used in burners and furnaces after a proper desulphurization and/or sold as a product.

The RC model is structured in order to represent the best available technologies (BATs). The flowsheet scheme of the RC model is shown in Figure 23. Accordingly to the considerations above, some decisions were taken for for the model:

Cogeneration

Although some plants still import electricity, this case was not considered. In fact, the benefits of cogeneration for this application are so evident that there is no reason not to install it in big plants.

The cogeneration unit is installed in the SAGD area and produces electricity for both extraction/processing and upgrading. The electricity is transported to the upgrading area via grid. The decision to place the cogeneration system in the SAGD area is due to the necessity of remaining close to the wells for steam production.

The cogeneration system will consist of gas turbines with once through heat recovery steam generators (OT-HRSGs). These particular systems produce steam with around 80% quality. Due to the impurities in the water, which is coming from the CPF, is not possible to use drum evaporators. In order to keep the liquid in contact to the pipes, it is mandatory to maintain low steam quality. If a complete evaporation occurs, the harnesses in the water could deposit over the surface of the pipes, creating fouling and several problems related. The power output selected for each unit is around 50 MW. As we mentioned, due to the severe climate in Alberta, it is generally preferred to use small size turbines.

Steam generation

All the steam generated is generated close to the users. The steam for the extraction is generated into the extraction area and the steam for the upgrading in the upgrading area. The HP steam for the wells, except the one from the cogeneration unit, is generated via OTSGs.

The superheated steam requested by the delayed coker is generated by the natural gas steam reformer used in the hydrogen production.

The saturated steam required by the stripping units is generated by drum boilers.



Figure 23: Flowsheet for the RC Model

Use of fuel products

All the gaseous hydrocarbons produced in the processes are desulphurized and used as fuels. The gas produced in the wells is used into the OTSGs as co-fuel with natural gas and in the post-firing system. The gas produced during the upgrading process is used in the drum boilers, in the steam reformers burners, and in the furnaces that provide heat to the upgrading units.

The extra gas is sold to the market. It is inconvenient to transport the extra gas from the upgrading to the extraction area due to the usual distance between them.

There is no use for the petcoke produced from the delayed coking, which is the actual situation of all the plants. A small amount of the petcoke produced is sold in the Asian market, while most of it is stockpiled.

3.2 FLOW SHEET MODEL

The calculation for the model has been done with the software Aspen Plus version 7.3 from Aspentech [29].

The main sheet of the Aspen Plus model of the SAGD extraction utilities consists in two main macro-areas:

- SAGD Extraction area
- Bitumen upgrading to SCO area

The first one is divided into:

- Cogeneration (COGEN)
- Mixed fuel OTSGs (OTSGs)

The upgrading is divided into:

- Steam reformers (SREF)
- Drum boilers (DB)
- Furnaces (FURN)

The main sheet of the Aspen RC model is shown in Figure 24. The inputs for the model are:

- Electricity demand
- Produced gas from wells and fuel gas from upgrading production
- HP steam required from wells of SAGD
- Hydrogen required
- Superheated steam required from upgrading
- Saturated steam required from upgrading
- Heat/fuel gas demand for furnaces


Figure 24:Flowsheet model of SAGD extraction energy facilities

All these quantities were defined and calculated in Chapter 3. The outputs of the model are:

- Natural gas consumption
- Electricity export
- Fuel gas to sell
- CO2 emissions

3.3 COGENERATION MODEL

3.3.1 Gas Turbine performance data corrections

In SAGD plants it is usually preferred to modularize the Electricity production using more small/medium size units than only one big unit.

This approach permits more flexibility in the case of change of production of bitumen, or to stop for maintenance of the units.

The gas turbines have been selected from the large number of machines available on the market. The final decision was to take the commercial 47.5 Mwe SGT-800 model from Siemens [32]. This model was selected mainly for two reasons. The first one is that the turbine output is the perfect size of the turbines usually used in SAGD plants. The second reason is that this specific model combines high efficiency with the high temperature of the exhaust gases, which is a good parameter for cogeneration use. The technical specifications for this machine are taken from the database of the software GT-PRO Version 18 from Thermoflow [33]. Since the new version of the gas-turbine is not available in the database the model of 2008 was used, which is very similar. A first simulation with GT-PRO was run and the results shown in Table 17 were obtained. The results of this simulation are referred to ISO conditions (15°C, 1 Atm) and do not consider pressure drops in aspiration and exhaust. Since the climate conditions in the Athabasca region of Alberta are extremely severe, and since some pressure losses are inescapable, another simulation for the 'Corrected site' conditions was done. These values were assumed for temperature and pressure drops:

- Annual average temperature 0°C
- Aspiration pressure drop $\Delta p_{asp} = 5$ mbar
- Exhaust pressure drop $\Delta p_{exh} = 20$ mbar

These values were used as an input in GTPRO for a new simulation. The results shown in Table 17 demonstrate that the corrections of the performance data are mandatory when the turbine is working in extreme temperature conditions like in Alberta.

Parameter	Unit	ISO conditions	Corrected site conditions
Power	MW	46.43	48.93
Efficiency	%	37.54	37.36
Air mass flow rate	kg/s	128.5	134.35
Fuel mass flow rate	Kg/s	2.5	2.65
Flue gas mass flow	kg/s	131.1	137
TIT	°C	1287.8	1292.9
Turbine outlet (TOT)	°C	551,82	540.8

Table 17: ISO conditions and Corrected site conditions for a Gas turbine SIEMENS SGT-800 in Alberta

3.3.2 Cogeneration Unit model

The cogeneration unit has been modeled with Aspen plus.

For the gas turbine, since all the data are already available, an equivalent model has been used. This model is used just to provide the composition of the flue gases in order to simulate a correct exchange in the OT-HRSG.

Those streams are sent to an RStoic block that simulates the combustion and its products. RStoic block is modeling a reactor when the stoichiometry is known.

Parameter-ID	Name	Yield (%wt)
C1	Methane	95
C2	Ethane	3.2
C3	Propane	0.2
iC4	Iso-butane	0.03
nC4	N-butane	0.03
C5+	Pentane +	0.02
02	Oxygen	0.02
N2	Nitrogen	1
CO2	Carbon Dioxide	0.5

Table	18:	Natural	Gas	composition	from	(23)
1 ant	10.	1 Jacul al	Gub	composition	nom	(20)

This block is modeled as an adiabatic reactor with no pressure drops. Furthermore, the option within the block to simulate combustion reactions was selected.

The exhaust gases are cooled down with a cooler block till the temperature EXT calculated in the former section (511.82 $^{\circ}$ C).

The exhaust gases are then post fired. The postfiring system has been modeled with another RStoic reactor that is receiving another inlet stream of fuel. Since the combustion in a gas turbine occurs with a large excess of air, the gases are still full of oxygen and can handle another combustion. The limit to the amount of fuel injected for the postfiring is the maximum temperature tolerable by the materials. The amount of fuel injected for postfiring was calculated with an iterative Design-Spec calculation, fixing 750 °C as maximum temperature. A mixed fuel, which is a mixture of natural and produced gas, was used in the postfiring unit.

The posfired stream is then sent to a heat exchanger that is simulating the OT-HRSG. The OT-HRSG is producing saturated steam at 100 bar with a vapour fraction of 78% [24].The heat exchange process has been simulated with a minimum temperature approach of 20°C and thermal losses of 1%.

The water and the steam produced by the OT-HRSG are then separated into a separator block. The steam is sent to the wells while the water is preheating the Boiling feed water. The Boiling feed water has a temperature of 166°C [24].

This steam is preheated with the water blow down from the separator until a temperature of 200°C. This heat exchanger has been modeled with a minimum temperature approach of 10°C.

The cogeneration unit is shown in Figure 25, while the Aspen cogeneration model is shown in Figure 26.

The input received by this unit is essentially the total electricity demand. The electricity demand profile of this process is not known. Since many similar industrial process have a constant demand profile, the plant was considered operative 24 hours a day. Therefore, the mean power demand results:

$$PD = Power \ Demand = ED * \frac{1}{24*1000} \ [MW] \tag{3.1}$$

$$NUMGT = NUMber of Gas Turbines = INTSUP(\frac{PD}{NR})$$
(3.2)

with NP = Nominal Power of SGT-800 = 51.27 [MW] (3.3)

Nevertheless, Gas Turbines have some inescapable stoppages due to maintenance and failures. The entire system won't be oversized basing on availability factors. When there is a shutdown of the gas turbine, the electricity will be bought from the grid. Hopefully, thanks to the modularization of the units, just a small part of the electricity required will be integrated in these situations. The steam produced by cogeneration will be reduced, and therefore, there will be an increase in the OTSGs load during the temporary stop. During normal operations the extra electricity, if any, will be exported to the grid. The cogeneration model is based on a single gas turbine but can easily handle more units. In fact, in the main sheet there is a multiplier block that can receive as an input the number of turbines that are operating in the SAGD plant. This unit multiplies the flow of gases for the number of machines. With this modification the air in the burners will be regulated by a calculator block. The OT-HRSG will be simulated as a single big unit that is receiving all the flue gases from the turbines and that is perfectly equivalent to the simulation of more OT-HRSGs. All the parameters used in the Aspen Model are displayed in Table 19.



Figure 25: Flowsheet of the Cogeneration unit

3.4 OTSGs MODEL

The OTSGs were modeled with an RStoic block and a heat exchanger.

The RStoic block is receiving air and fuel and is simulating an adiabatic combustion without pressure drops. The air flow rate is set with a design spec in order to have 3% of oxygen in dry flue gases.

The heat exchanger receives the gases at the flame temperature and produces water at 100 bar and 78% quality.

The minimum approach temperature is 20°C. The losses are set to be 0.5% of LHV for unburned and 0,5 of LHV for radiation and convection losses.

As for the cogeneration unit, the stream exiting the OTSG is separated into steam and water, which is preheating the feedwater of the boiler.

The heat exchanger for the boiler feedwater is identical to the one described in the former section for cogeneration. The pure steam produced at 100bar is sent to the wells and it is used for the extraction.

The OTSGs model is shown in Figure 27.

Table 19: Parameters for Steam Generation

Parameter	Unit	Value
Natural gas consumption for each Turbine	Kg/s	2.734
Mass of air for each turbine	Kg/s	136.01
Turbine Exhaust temperature	°C	551.82
Postfire Temperature	°C	750
Temperature Water Preheat inlet	°C	166
Pressure water preheater inlet	bar	135
Minimum Temperature Approach in Water preaheater	°C	10
OT-HRSGs Heat Losses	%	1
Quality of OT-HRSG	%	78
Outlet Steam pressure	Bar	100
Minimum Temperature Approach OT-HRSG	°C	25
Air Inlet temperature Burners OTSGs	°C	25
Oxygen Mole fraction in Dry gases	%	3
Losses for unburnt	% of LHV	0.5
Losses for radiation	% of LHV	0.5
Quality of OTSGs	%	78
Outlet Steam pressure	Bar	100
Minimum Temperature Approach OTSG	°C	25



Figure 26: Cogeneration model



Figure 27:OTSGs model

3.5 STEAM REFORMERS

For the hydrogen production, a natural gas steam reformer unit was modeled with Aspen Plus. Particular effort was dedicated in order to make a proper model of this unit. The model consists in a pre-reforming unit, a steam reformer unit, two stages of water gas shift (WGS) and a pressure swing adsorber (PSA) for hydrogen purification. The flow diagram of the steam reformer modeled in this section is shown in Figure 28.

Since the natural gas considered in the models doesn't contain H_2S , no desulphurization was included before the reactors.

Nevertheless, in commercial plants a desulfurization unit with a zinc oxide bed is always required because of the low tolerance of catalysts for sulphur.

The main reactions involved in the Natural gas Steam reforming are [34]:

- $CH_4 + H_2O \rightarrow CO + 3H_2$ $\Delta H_{298}^0 = 206 \text{ KJ/kmol}$
- $CO + H_2O \rightarrow CO_2 + H_2$ $\Delta H_{298}^0 = -41 \text{ KJ/kmol}$
- $CH_4 + CO_2 \rightarrow 2CO + 2H_2$ $\Delta H^0_{298} = 247 \text{ KJ/kmol}$
- $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$ $\Delta H_{298}^0 = 165 \text{ KJ/kmol}$

•
$$CH_4 + 3CO_2 \rightarrow 4CO + 2H_2O$$
 $\Delta H^0_{298} = 330 \text{ KJ/kmol}$

All the reactions are taking place in the steam reformer reactor, except the second, the WGS reaction, which is happening in the WGS Reactor.

The reactions taking place in the Steam reformer reactor are overall endothermic. Because of that, burners are required in order to supply external heat to the reactor. The main goal of this process is to convert as much as possible the inlet Natural gas into Hydrogen. The reactions are promoted at a high temperature and low pressure. In order to do that, the temperature of the reactors should be as high as possible. A general limit is represented by the resistance of materials to 900-920°C [35]. Although a low pressure is positive for the thermodynamic, it is mandatory to limit the dimensions of the reactors. In addition, the final product is required to be pressurized, and it is absolutely inconvenient to compress the gaseous products.

The usual range of pressure of these units is between 20 and 40 bars.

Another parameter that is positively affecting the conversion of methane is the Steam to CH4 rate. Generally it is recommended to operate with rates between 2.5 and 4. A higher amount of Steam is reducing the Methane slip and is also preventing the accumulation of solid carbon that is negative for the catalyst and the pipes.

The parameters used for the steam reformer reactor are an outlet temperature of 900 $^{\circ}$ C, a pressure of 38.5 bar and a steam to CH₄ ratio of 2.7.

The refinery requires pure hydrogen while the Syngas produced in the reforming reactor has a discrete content of CO.



Figure 28: Steam reformer flow diagram



Figure 29:Steam Reforming Model

Because of that, WGS reactors are installed in order to convert the CO to H2 and CO2 with the remaining Steam water in the syngas flux.

Typically two shift reactors are used: The first one is operating with high temperature catalysts, while the second operates with low temperature catalysts.

The first reactor is operating with iron oxide– chromium oxide catalysts with a usual inlet temperature of 300-450 °C. The second reactor uses Cu-ZnO-Al₂O₃ catalysts that usually operates in a range of 190-250 °C [36].

The inlet temperatures for HTS and LTS reactors are respectively 400 and 200 $^{\circ}$ C (Figure 30).



Since the reaction is exothermic, the flux of syngas out of the high temperature shift (HTS) has a higher temperature than the one entering the reactor.

The syngas flux is then cooled down in a heat exchanger until the desired temperature for the low temperature shift reactor (LTS) has been reached.

The main sheet of the steam reformer model is shown in Figure 29.

For the steam reforming and WSG reactors an RGibbs block has been used.

RGibbs models single-phase chemical equilibrium, or simultaneous phase and chemical equilibria. It must be specified the reactor temperature and pressure, or pressure and enthalpy. RGibbs minimizes Gibbs free energy, subject to atom balance constraints. This model does not require reaction stoichiometry. RGibbs can determine phase equilibrium without chemical reaction.

For the Steam reformer unit, all the components were selected as possible products. No components were considered inerts.

In the case of the WGSs, all the components were considered inerts except the ones involved in the shift reaction. The shift reactor is simulated as adiabatic.

An adiabatic pre-reformer unit is also included in the scheme. This unit is not mandatory in the case of usage of natural gas as a feed, although it is mandatory when heavier hydrocarbons are processed.

The reactions involved are the same described above plus the generic reforming reaction:

 $C_n H_{2n+2} + n H_2 O \longrightarrow n CO + (2n+1) H_2$

The use of the pre-reformer can also have a positive impact when the feed is natural gas. In fact, the pre-reformer can reduce the thermal load of the steam reformer, the steam to CH4 ratio and increase the overall efficiency of the process [35].

This unit was simulated as an adiabatic RGibbs block with the same characteristics of the Steam reformer.

After the second shift the syngas is cooled down and sent to the purification units. The hydrogen in the syngas should be separated from the other components in order to obtain the desired purity.

After the separation of the water, the syngas is sent to a pressure swing absorber (PSA). The PSA has been modelled as a simple separator block set to recover 90% of hydrogen with 99.99% of purity. This block has been used on the basis that hydrogen purity and recovery are not sensitive to the changes in pressure and composition of the feed [37]. The hydrogen produced is sent to the hydrotreates while the Offgas of the PSA, which is mainly composed of CO2, H2, CH4, CO and H2O, is sent to the burners of the SRR.

The burners of the steam reforming are modeled in a separate model that is shown in Figure 31.

The Steam reformer burners are using as a fuel the offgas from the PSA and some gas produced in the Upgrading Process.

The burners were modeled with an adiabatic RStoic unit that generates the combustion reactions. After the burner there is a control model that verifies the concentration of O2 in the exhaust gases. A concentration of 3% O2 in dry gases was fixed.

The exhaust gases are then cooled down, providing heat not just to the steam reformer reactor but also to other streams. In fact, a system of heat exchangers was created. This system is similar to the scheme illustrated in [35]

The exhaust gases are therefore preheating the feed of the steam reformer, the natural gas feed, and the air of the burners. There is also some steam generation with the heat of the exhaust gases. The heat exchangers are set with 0.5 % heat losses and minimum temperature approach depending on the different currents. The heat for steam production is also provided from the syngas coolers after the reforming reactors and the WGS reactors. The heat at high temperature is used to produce steam while the heat at low temperature is used for water preheating.



Figure 31:Steam reformer Burners and Heat Exchangers Model

The steam is produced at 38.5 bar and 500°C. Some of this steam is used for the reactor while the remaining is exported to the delayed coker.

The steam production model is shown in Figure 32.

The parameters used for simulating the plant are displayed in Table 20 while the performances of the plant are shown in Table 21.

Parameter	Unit	Value
Natural gas Pre-heater outlet temperature	°C	500
Superheated Steam Temperature at mixer	°C	500
Inlet pressure	bar	38,5
Steam to Methane Ratio	Mol/Mol	2,7
Pre Reformer feed temperature	°C	500
Pre Reformer Heat Duty	MW	0
Pre Reformer Pressure Drop	bar	1
Steam Reformer Feed Temperature	°C	650
Steam Reformer Outlet Temperature	°C	900
Steam Reformer Pressure Drops	bar	1
High Temperature Shift inlet Temperature	°C	400
HTS Heat Duty	MW	0
HTS pressure Drops	bar	0.5
Low Temperature Shift inlet Temperature	°C	200
LTS Heat Duty	MW	0
LTS pressure Drops	bar	0.5
HTS/LTS reactor approach temperatures	°C	10
Condenser Temperature	°C	40
PSA inlet Temperature	°C	40
PSA Hydrogen Split fraction	%	0.9
PSA hydrogen Quality	%	1
Combustion Air Temperature	°C	425
O2 Concentration in Dry Gases	%	3
Minimum Approach temperature Exhaust Gases/Syngas Exchangers	°C	100
Minimum Approach Temperature Syngas/water exchangers	°C	25

Table 20: Parameters for the Steam Reformer

Exhaust Gases Outlet temperature	°C	215
Heat Losses from heat exchangers	%	0.5
Pressure Drops in Heat exchangers Gas side	%	0.05

The efficiency is calculated with these equations:

$$\eta_{1} = \frac{\dot{m}_{H2}*LHV_{H2}}{\dot{m}_{NG}*LHV_{NG} + \dot{m}_{FUEL}*LHV_{FUEL}}$$

$$\eta_{2} = \frac{\dot{m}_{H2}*LHV_{H2} + \dot{m}_{STEAM-EXP}*\Delta H_{@38.5bar,500^{\circ}C}}{\dot{m}_{NG}*LHV_{NG} + \dot{m}_{FUEL}*LHV_{FUEL}}$$

$$(3.4)$$

Where :

 \dot{m}_{H2} , $LHV_{H2} = Mass$ Flow rate and LHV of Hydrogen \dot{m}_{FUEL} , $LHV_{FUEL} = Mass$ Flow rate and LHV of the fuel of the burners \dot{m}_{NG} , $LHV_{NG} = Mass$ Flow rate and LHV of Natural Gas $\dot{m}_{STEAM-EXP}$, $\Delta H_{@38.5bar,500°C} = Mass$ flow rate and specific variation of enthalpy of the steam produced for the export

 $\eta_1 = Efficiency of the Steam Reformer$

 $\eta_2 = Efficiency of the Steam Reformer (Steam Export included)$

The inputs for the steam reforming unit were essentially the demand of natural gas from the HTRs and the amount of steam required from the delayed coking unit. This 'type' of steam was selected because it has characteristics similar to the steam required from the steam reforming.

In order to reach exactly the values required by the demand, a design spec flowsheeting option was used.

In the case of hydrogen production, the flowsheeting option is varying iteratively the input of natural Gas in order to produce the hydrogen required.

The values of steam produced by the steam reformer have been reached working on the heat exchangers flows.

Parameter	Unit	Value
Natural gas Steam reforming consumption	Kg/s	8.23
	MW	404.72

Table 21: Performances of the Steam Reforming Unit

Fuel Gas Consumption	Kg/s	0.49
	MW	23.68
H2 produced	Kg/s	2.65
	MW	317.89
Superheated Steam at 500°C and 38.5 bar exported	Kg/s	16.11
	MW	55.71
Efficiency η_1	%	74.19
Efficiency η_2 (Steam Production included)	%	87.19



Figure 32:Steam Reformer Steam Generation Model

3.6 DRUM BOILERS AND FURNACES

The drum boilers and furnaces hierarchies complete the upgrading area.

drum boilers are producing the steam required for stripping in the DRU and hydrotreating. They essentially receive saturated liquid at 20 bar and produce a complete evaporation of the liquid flow by burning fuel gas produced by upgrading.

The simplified drum boilers model in Aspen is not very different than the one made for OTSGs (while in reality those units are extremely different from each other). The main difference is that these units, thanks to their structure, are producing saturated steam with

around 100% quality. Thus, they don't require a flash separator as OTSGs do in order to produce pure saturated steam.

Therefore, their results are more economical and efficient than OTSGs.

The furnaces are producing the heat required by the heaters in the different upgrading units. Since Gary's [20] value for fuel requirements is already comprehensive of the combustion efficiency, the modeling of furnaces is not required. The fuel requirements can be calculated with only one simple equation:

$$\dot{m}_{FUEL} = \frac{FD}{LHV_{FUEL}} \tag{3.6}$$

Where FD is the Fuel demand, \dot{m}_{FUEL} and LHV_{FUEL} are the mass flow rate and LHV of the fuel of the furnaces.

Nevertheless, an equivalent model has been simulated in order to predict the CO₂ emissions. An RStoic combustor has been modeled with an input of fuel equal to \dot{m}_{FUEL} . After the combustion, the heat exchange has been simulated without any loss in order to produce exactly the heat demand FD. Although this model box does not provide us with any additional information, it is required to maintain the structure of the model and calculate additional streams. These additional streams are the CO₂ emissions and the extra fuel which is not used in the upgrading burners and is available for sale. The parameters of the drum boilers model are shown in Table 22.

Parameter	Unit	Value
Air inlet temperature burners DB	°C	25
Oxygen mole fraction in dry gases	%	3
Losses for unburnt	% of LHV	0.5
Losses for radiation	% of LHV	0.5
Quality of DB	%	100
Outlet steam pressure	Bar	20
Minimum temperature approach DB	°C	20

 Table 22: Drum Boilers Parameters

3.7 OTHER UNITS

There are a few more units in the main sheet that haven't been described yet. In both SAGD extraction and upgrading area there is a sweetening unit. For desulphurization, a Sulfinol process was selected. This process is the one used by Suncor in Athabasca region [17]. The sweetening units have been modeled in Aspen Plus as a simple separator block that separates all the H_2S and part of the CO_2 from the inlet feed. The solvent should then be regenerated with reboiling/stripping with steam. There is a certain heat required for the reboiling and a certain amount of electricity required for the AGR. However, since these values are extremely low compared to the other streams involved in the model, they are considered negligible. The H_2S is sent to the Claus facility, where elemental sulphur is produced while the CO_2 is vented in the atmosphere. The mixing unit blends natural and sweet produced gas. That operation is done mainly because the sweet produced gas has a lower heating value than the natural gas. A feed with just sweet produced gas could require some modification to the conventional burners of the OTSG, which is undesirable.

The mixed gas then enters into a split unit that divides the fluxes between postfiring and OTSGs. This unit is controlled by a design spec that sends to the cogeneration model the mix-fuel necessary for the postfiring system in order to respect the temperature limits (Section 3.3.2).

3.8 RESULTS

In this section, the main results of the model for the reference case are discussed. First of all, the specific consumption of energy of the various units was calculated and compared. With these data a net energy analysis (NEA) of the energy system was performed. In order to do that, some parameters called energy return ratio (ERRs) have been used.

In the end, the CO2 emission of the RC were calculated. These results have been compared to the ones of other studies available in the literature.

The flowsheet with results for the RC model is shown in Figure 33.

3.8.1 Energy consumption in the RC model

In the RC model the energy is provided to the energy facilities with gaseous fuels. The gaseous fuels used in the SCO life cycle (LC) are natural gas (NG), produced gas from wells (PG) and fuel gas (FG) from coker.

A specific consumption of fuel was attributed to every unit. In most of the cases the attribution of fuel consumption to each unit was easy, but for the cogeneration unit the process was not so simple. In fact this unit produces energy streams for different purposes:

- Electricity for SAGD
- Electricity for upgrading
- Electricity for export
- Steam generation for SAGD

It has been decided that the natural gas consumption for electricity generation is the fuel used in the simple cycle of the gas turbine. Therefore, each electricity stream has a consumption of natural gas proportional to its electricity production.



Chapter 3

Figure 33: Flowsheet with results for the RC model

The stream of steam generated for SAGD is associated with the fuel used for the postfiring in the OT-HRSGs.

As described in Chapter 3, two scenarios for the SAGD extraction were performed. The first scenario corresponds to a low energy Scenario (LES), with a SOR of 2 and EOR of 7.5. The second scenario corresponds to a high energy scenario (HES), with SOR of 3 and EOR of 14.

The results of the two different simulations with Aspen Plus are shown in Table 23. As can noticed from the results, the SAGD area relies majorly on natural gas use, while in the upgrading area the fuel gas produced gives a significant contribution.

The units that consume more energy are without any doubt the OTSGs followed by the furnaces of the upgrader reactors and the steam reformer. In the LES the energy consumption is almost equally divided between extraction and upgrading. In this case the consumption of OTSGs is almost the same of the sum of furnaces and steam reformers. Moreover, the natural gas consumption for electricity generation is equally ascribable to SAGD and upgrading.

However, in the HES the results are very different. In this case the SAGD area is consuming 70% more energy than the upgrading area. This is attributable mainly to the high increase of steam demand from the wells, which is definitely the most influent parameter on the entire process.

3.8.2 Net energy analysis

Net Energy Analysis (NEA) is a class of methods used to calculate the effectiveness of energy systems [38] .These methods are particularly effective whenever there is the extraction or the exploitation of natural resources.

In these cases, it's not just important to find a parameter who measures the thermodynamic efficiency of the energy conversion. In fact, it does matter to evaluate in terms of energy how profitable it is to exploit a natural resource (as for example are hydrocarbons). The result of a NEA is usually an energy return ratio (ERR), a parameter which compares the amount of energy consumed in exploitation of an energy resource to the amount of valuable energy provided to society.

Interesting considerations can be made through the analysis of the ERRs parameters. These parameters, contrary to the thermodynamic efficiencies, should be always bigger than one. If not, it means that it costs us more energy to extract a resource than the energy this resource provides to users.

There are a lot of formulations of ERRs. Each of these formulations provides different information, depending also on the boundaries used.

Since ERRS are often poorly defined in the literature, it was decided to refer to the work of Brandt and Dale [39], who brilliantly defined some ERRS.

The Net Energy Ratio (NER) considers all the energy input for the process, and its general formulation is:

$$NER = \frac{Net \ Output \ of \ Primary \ Energy}{External \ Primary \ Energy+Self \ Consumption \ Primary \ Energy}$$
(3.7)

The net external energy ratio (NEER) considers only those inputs that are 'consumed from the existing industrial energy system, excluding any self use (e.g. produced oil burned on site to power oil producing operations)'. Its general formulation is:

$$NEER = \frac{Net \ Output of \ Primary \ Energy}{External \ Primary \ Energy}$$
(3.8)

The ERR type 'external' with the 'flow' formulation defined by Brandt and Dale [39] was selected for this analysis. This ERR type, contrary to the 'Life Cycle' type, does not consider any indirect energy use. Indirect energy uses are, for example, the energy consumption associated to natural gas bought from plants or the energy used in order to build the energy facilities.

Generally speaking, the NER parameter is a measure of the total return from a certain production process. This parameter is closely correlated with the environmental impacts of a process (like greenhouse gas emissions).

Conversely, the NEER can measure the potential growth in energy supply to society because it only counts those inputs that must be produced and delivered externally to the process through the existing energy supply system.

Therefore it is useful to compare these parameters in order to have a complete overview on the energy profitability of the process. This comparison indicates to what extent a certain process is energetically independent. The ERRs and streams used for their calculation are shown in Table 24. The SCO production, the fuel and the electricity export have been considered as energy outputs. Since the electricity is not a primary energy, we have to convert it. The benefit that this exported electricity is providing to society is saving in fuel, that otherwise would have been consumed from electricity grid producers. In order to make a fair calculation, the mean efficiency of conversion of Alberta's electric grid was taken from [40]. The conversion in terms of primary energy for the electricity is:

$$Primary \ energy_{electricity \ exp} = \frac{Electricity \ export}{\eta_{el-ALBERTA}}$$
(3.8)

Where $\eta_{el-ALBERTA} = 0.4$ is the mean electric efficiency in Alberta

The only external energy input is natural gas bought from the pipeline. The self consumption of energy refers to the gases produced during the processes. A range of values of 3.02-3.9 was obtained for the NER and a range of 3.85-5.42 for the NEER. In another study applied on the oil sands industry, Brandt [41] calculated the values of NER and NEER over the years for in situ extraction process. The values for in situ calculated by Brandt are around 3.3 for NER and 4.5 for NEER.

Block	NG (LES)	NG (HES)	PG	FG	Energy (LES)	Energy (HES)
	kg/s	kg/s	kg/s	kg/s	MM	MW
COGEN	6.80	10.24	0.00	0.00	337.39	506.05
ELESAGD	2.50	4.66	0.00	0.00	122.76	229.13
ELEUPGR	2.59	2.59	0.00	0.00	127.24	127.24
ELEEXP	0.38	0.94	0.00	0.00	18.51	46.40
SGCOG	1.34	2.05	0.20	0.00	68.88	103.29
OTSGs	22.58	34.55	3.41	00.0	1160.93	1739.58
SR	8.23	8.23	0.00	0.49	428.40	428.40
DB	0.00	0.00	0.00	0.75	36.15	36.15
FURNACES	0.00	0.00	0.00	13.30	637.73	637.73
SAGD	26.60	41.73	3.61	0.00	1361.81	2095.19
UPGRADING	11.01	11.29	0.00	14.55	1238.78	1252.72
TOT	37.61	53.02	3.61	14.55	2600.59	3347.91

 Table 23: Energy Consumption of the RC Model

This data refers only to the extraction process and doesn't take into account the upgrading to SCO of in situ bitumen. The upgrading of bitumen consumes a significant amount of energy but most of it occurs within the process (self consumption). This means that the value of NER should decrease sharply, while the NEER should maintain a similar value. Because of that, Brandt calculates a measure significantly lower than us of the NER. A possible explanation is that, within the period of interest that he considered, the values of SOR he had used were higher than the values used in the demand prediction model.

Parameter	Unit	LES ¹	HES ²
SCO Production	kg/s	204,24	204,24
	MW	9505,47	9505,47
Fuel gas export	kg/s	8,28	8,28
	MW	396,89	396,89
Electricity export	MW	2.39	10.7
Electricity export in primary energy	MW	5.97 ³	26.75
Natural gas consumption	kg/s	37,61	53,02
	MW	1829,67	2576,99
Produced gas consumption	Kg/s	3,61	3,61
	MW	73,36	73,36
Fuel gas consumption	Kg/s	14.55	14.55
	MW	637,73	637,73
NER	GJ _{out} /GJ _{in}	3,90	3,02
NEER	GJ _{out} /GJ _{in}	5,42	3,85

Table 24: Main energy streams and ERRs of SCO production for the reference case

1 LES refers to low energy scenario, with SOR of 2 and EOR of 7.5

 $2\ \mathrm{HES}$ refers to high energy scenario, with SOR of 3 and EOR of 14

3 An efficiency of 0.4 has been taken for Alberta's electric grid

The result of Brandt would have probably been close to the one obtained in this study, if similar values of SOR had been used.

However, these values are very far from the values of NER of conventional oil resources. According to Brandt, conventional oil NER ranges from 15 to 30 GJ/GJ [41].

Generally speaking, it means that a use of 1 GJ of energy produces around 5 GJ of SCO. Likewise, with the same input of energy it could be produced more than 15 GJ of conventional crude.

These numbers are showing how energy intensive this process is and how it is less profitable than the conventional extraction.

3.8.3 CO2 emissions

In this section, the CO_2 emissions for the reference case are calculated. The emissions calculated are specific for every unit. For the cogeneration unit, the same criteria used for energy consumption were used: The CO_2 emissions for electricity production are related to the gas turbine simple cycle combustion. The CO_2 emissions related to the steam cogeneration are ascribable to the postfiring.

However, the export of electricity shouldn't be counted totally into the emissions of CO_2 . In fact, the export of electricity contributes to a reduction in the electricity production of Alberta's electrical grid. The reduction in CO_2 emissions is equivalent to the electrical grid emissions to produce this amount of electricity. The value of mean CO_2 emission of the electrical grid is 750 kg CO_2/MWh and has been taken from [40]. This value has been subtracted from the total emissions.

The results obtained are shown in Table 25.

The same comments made for energy consumption can be made for CO_2 emissions. In the LES the emissions produced in the SAGD and in the upgrading are similar. In the HES the emissions produced from the SAGD area are far superior (+65%).

As can be seen from Table 23 and 25, the utilities that consume more energy also produce more emissions. This result derives from the fact that the fuels used in the processes have a similar carbon content (The FG has a slightly higher carbon content) and tendency to produce CO₂.

The model calculates only the direct emissions associated to the energy production of the unit. There are no emissions calculated for the transport between SAGD and upgrading of electricity and dilbit.

The results in Table 25 are expressed in absolute flow (kg/s) or relatively to the product generated (bitumen or SCO).

The results are then compared with Charpenter's GHOST model [3]. The comparison of values obtained by the two models is shown in Table 26.

The CO₂ emissions values are very similar between the two models. The GHOST range values for the SAGD extraction are slightly higher than the on of this model. This is explainable mainly because in the GHOST model, the range of SOR is 2.3-3.3 (Here, a range of 2-3 was used). The GHOST model also simulates two scenarios (low and high energy use) for the upgrading. The wide range of values obtained for the upgrading emissions is mainly due to the uncertainty of the author about the hydrogen consumption of the HTRs [3]. However, the value obtained fits perfectly in the range calculated by GHOST model.

UNIT	LES ¹	HES ²	LES	HES	LES	HES
	kg/s	kg/s	g/MJ _{BIT}	g/MJ _{BIT}	g/MJ _{SCO}	g/MJ _{SCO}
SWEET	0.61	0.61	0.05	0.05		
COGEN	18.86	28.24	0.98	1.68	0.73	0.73
EleSAGD	6.83	12.75	0.58	1.08		
Eleupgr	7.08	7.079			0.73	0.73
Eleexp	1.03	2.58				
Sgcogen	3.92	5.84	0.41	0.61		
OTSGs	66.36	98.61	6.88	10.22		
SR	23.57	23.57			2.44	2.44
DB	2.21	2.21			0.23	0.23
FURNACES	39.03	39.03			4.05	4.05
CO ₂ AVOIDED	1.47	3.69				
SAGD	77.5	117.26	7.92	11.96	8.06	12.21
UPGRADING	71.67	71.33			7.45	7.45
TOTLC	149.17	188.59			15.48	19.57

Table 25: CO2 Emissions of the RC Model

1 LES refers to low energy scenario, with SOR of 2 and EOR of 7.5

 $2\ \text{HES}$ refers to high energy scenario, with SOR of 3 and EOR of 14

Stage	Unit	RC		GHOST	
		LES ¹	HES ²	MIN	MAX
SAGD recovery and extraction	gCO2/MJ _{BIT}	7.92	11.96	8.4	12.3
Upgrading	gCO2/MJ _{SCO}	7.45	7.45	6.8	11.1
Total	gCO2/MJ _{SCO}	15.48	19.57	15.2	23.4

 $1\ \text{LES}$ refers to low energy scenario, with SOR of 2 and EOR of 7.5

2 HES refers to high energy scenario, with SOR of 3 and EOR of 14

CHAPTER 4: Modeling the gasification case

In this chapter, a model is simulated in order to satisfy the demand of energy calculated in Chapter 3.

The model simulated in this chapter, unlike the model developed in Chapter 3, consists in a gasification based polygeneration plant. The petcoke produced from the delayed coking is used as the fuel for the gasifier.

The gasification case (GC) was modeled with the software Aspen Plus from Aspentech [29]. The gasification solution selected, as it will be explained in Section 4.2.2 is the Shell/Prenflo technology of entrained flow gasifier.

Two gasification-based solutions are proposed:

- GC-VS (venting scenario): without CO2 capture (all CO2 is vented to the atmosphere)
- GC-CS (capture scenario): with CO₂ capture from syngas

4.1 STRUCTURE OF THE GASIFICATION CASE (GC)

In the GC, a polygeneration infrastructure is created. The gasification based polygeneration plant produces electricity, steam and hydrogen for the process.

The main product of the gasifier is the syngas, which is a mixture of CO, H_2 and traces of other incondensable gases. The syngas can be used in a gas turbine (with some modifications) for cogeneration. Furthermore, the syngas can be converted into H_2 through a shift reaction and the separation of the other components.

The gasification based polygeneration plant will provide all the pure hydrogen required from the hydrotreaters. Moreover, it will produce electricity for the processes and for the auxiliary components.

The steam required from the upgrading process will be generated from the syngas coolers. Some of the steam for the SAGD injection is produced by the OT-HRSGs of the gas turbines. In the GC-VS then, some high pressure steam for the wells is generated into the syngas coolers. Since this amount of steam will not be enough to satisfy the demand of the wells, some steam will be produced through OTSGs. The OTSGs will be fueled with sweet produced gas, natural gas and fuel gas produced in the upgrading.

Just in the GC-CS then, a natural gas fueled cogeneration plant is installed. This additional unit is required because the polygeneration plant cannot produce enough electricity for the processes.

The gasifier plant will use all the petcoke produced from delayed coking. This petcoke, in the RC (Chapter 4), was stockpiled without any use.



Figure 34: Flow sheet for the GC



Figure 35: : Main Aspen Flowsheet of the Gasification Case (GC)

In the GC, the heat required by the furnaces is produced by the fuel gas generated into the upgrading area. It is important to specify that in the GC the SAGD and upgrading areas cannot be very far one from the other.

This condition, which would also guarantee significant benefits in the RC, is absolutely mandatory in the GC.

The gasifier should be located close to the delayed coker, where the petcoke is produced. On the other hand, the high pressure steam for the extraction should be generated close to the SAGD wells. Thus, the turbines and the OTSGs have to be in the SAGD area. In the venting scenario then, a small amount of high pressure steam is generated into the syngas coolers. In the case of big distances between the two areas, the transport of the syngas from the upgrading to the SAGD would be very expensive. These factors could make the process less effective and anti-economical. Because of that, it is assumed that the upgrading is done close to the SAGD extraction and processing. This assumption leads to some other advantages. For example, the fuel gas produced during the upgrading can be used as a fuel for OTSGs.

This configuration is effectively adopted by CNOOC plant of Long Lake. This plant is installing a Shell gasifier alimented with asphaltanes. The configuration of the GC is very similar to the one adopted by CNOOC.

The flowsheet of the GC is shown in Figure 34, while the Aspen model's flowsheet in Figure 35.

4.2 SELECTION OF THE GASIFIER

In this Section, a proper gasification technology is selected for the GC.

In order to do that, the characteristics of the Athabasca bitumen petcoke will be analyzed in Section 4.2.1. The selection of the proper gasifier should be dependent on the bitumen characteristics.

Further, in Section 4.2.2, it will be explained why a Shell/Prenflo entrained flow gasifier was selected for this study. In this Section, a quick overview of this technology will be conducted.

4.2.1 Petcoke Characteristics

In order to select the appropriate technology of gasification, it is very important to analyze the properties of the oil sands petcoke.

In Furimsky's review [7], there is a complete analysis of the petcoke produced in the oil sands industry. The analysis includes the petcoke produced by delayed coking of Suncor and fluid coking of Syncrude.

The chemical properties of the petcokes are similar.

Essentially, the petcoke has a graphite-like structure, resulting from prolonged exposure to high temperatures. Compared to some coals used in commercial units, petcoke presents some differences:

- Higher level of fixed carbon, usually between 80 and 90% (same rank as anthracite coal)
- Lower levels of ash (between 3 and 8% for petcoke, much higher than 10% for Coal)
- Higher content of sulphur (usually around 2%, but for oil sands petcoke 5-7%)
- Moisture content is negligible compared to commercial coal

The characteristics of Suncor's petcoke are described in Table 27.

The high content of fixed carbon and the low content of ash raise the lower heating value of the petcoke to values similar to the highest rank anthracites.

Element	Value (%wt)			
Proximate Analysis				
Moisture	0.4			
Volatile	12.45			
Fixed carbon	83.37			
Ash	3.78			
Ultimate Analysis				
Carbon	83.7			
Hydrogen	3.7			
Nitrogen	1.8			
Chlorine	0			
Sulphur	5.7			
Oxygen	1.3			

 Table 27: Composition of Suncor's petcoke from [42]

Ash fusion temperature is another important parameter of the coke behavior during gasification. The gross heating value of Suncor petcoke along with the ash fusion temperatures is shown in Table 28.

Table 28: Heating value	s and ash fusion to	emperatures of S	uncor's coke	[7]
8		1		

Parameter	Unit	Value
Gross heating value	MJ/kg	35.157
Ash fusion temperatures		
Initial	°C	1074

Softening	°C	1285
Hemispherical	°C	1338
Fluid	°C	1446

The physical characteristics of the petcoke product are a very important parameter for preparing a good feedstock for the gasifier.

In this case, the products of fluid coking and delayed coking are very different from each other.

The produced coke from fluid coking is in powder form while the product of delayed coking is in the form of large lumps.

The particle size distribution of Suncor's delayed coking is shown in Table 29.

According to Furimsky [7], the reactivity of the coke of oil sands for gasification is low, and similar to the one of high rank coals such as anthracite.

Sieve range ¹	Diameter range ²	Content of fraction (wt%)
+4	d > 4.76 mm	2.5
- 4 to +14	1.4 mm < d < 4.7 mm	1
-14 to +20	841 μm< d < 1.4 mm	4
-20 to +60	250 μm < d < 841 μm	27.6
-60 to +100	149 μm < d < 250 μm	51
-100	d < 149 μm	12.9

Table 29 : Particle size distribution

1 Data taken from [42].

2 Conversion made from [43]

4.2.2Selection of Shell/Prenflo gasifier

In the literature, it is commonly agreed upon that entrained bed gasifiers are the best choice for oil sands petcoke [7].

Moving bed and fluid bed does not seem to be a good option for this case. According to Furimsky [7], the main limits for moving and fluid bed gasifiers are:

- The physical characteristics of oil sands petcoke do not seem to be suitable for those types of gasifiers. Some of the particles of Suncor's delayed coking are very small and contain fines (Table 29).
- Petroleum coke has relatively low reactivity. Because of that, high temperatures are required in order to achieve high gasification rates.

- Petroleum coke has a very high content of sulphur. In fluid bed gasifiers, limestone is usually used for in situ sulfur capture. However, in this case an amount of limestone up to 4 times the amount used for conventional coke should be used.
- It is uncertain whether the solids produced could meet the requirements for nonhazardous wastes

Although maybe fluid or moving bed gasifiers could be used with some modifications, the performances may not be as good as those of entrained bed gasifiers. Regarding the problems listed above, entrained bed gasifiers seem to be the best option because of these reasons:

- Although the particle size needs to be reduced to less than 100 μ m for entrained flow gasifiers, this can be done easily in a grinding system.
- Entrained bed gasifiers are operating with very high temperatures (approaching 1500°C). This parameter ensures a very high gasification rate.
- Sulphur removal is done in the syngas treatment, after the gasification, and is absolutely not problematic.
- Entrained flow gasifiers then produce a syngas of exceptional quality, clean and tar-free.

However, for entrained bed gasifiers it is mandatory to use pure oxygen instead of air. Thus, a cryogenic air separation unit (ASU) has to be installed. Although this unit is wellknown and mature, it is also very expensive in terms of capital cost and auxiliary power required.(Section 4.9)

According to Furimsky [7], both Shell and Texaco indicate Suncor coke as an ideal feedstock for their technology.

The GEE process (previously Texaco) uses slurry feed downflow entrained flow gasifiers. The reactor shell is an uncooled refractory lined vessel.

The solution for the syngas cooling can be a radiant boiler, a water complete quench or a combination of the two.

Accordingly to Higman [44], the GEE process is without any doubt the least expensive technology on the market. Furthermore, the water quench is particularly suitable for chemical applications such as the making of ammonia and hydrogen.

However, steam is the most influential energy vector in the process and it is desirable to maximize its production. Although the GEE process could have been a good selection, choosing a solution that produces more steam was preferred, as the Shell/Prenflo does.

The Shell/ Prenflo (pressurized entrained flow) solution consists of a dry feed upflow reactor with a membrane wall vessel. The syngas is cooled to 900 °C with a recycled cold syngas quench. After the syngas quench, which recycles almost 50% of the syngas, the syngas is cooled to around 250-280°C, producing steam.

A variant of the syngas coolers recently introduced for this reactor is the water quench. The Shell/Prenflo solution technology is more expensive than the GEE one, because of the higher capital cost of the membrane wall, the syngas quench and the syngas coolers.

Nevertheless, since the Shell solution is a dry coal feed gasifier, it has a consumption of oxygen 20-25 % lower than the slurry feed gasifier [44]. Since the auxiliary power request of the ASU is proportional to the oxygen consumption, a reduction of the oxygen consumption leads to a consistent increase in efficiency.

4.3 FLOW SHEET MODEL

The main sheet of the Aspen Plus gasification model essentially consists in four facilities:

- Gasification based polygeneration plant
- Additional natural gas fueled cogenerations (For capture scenario GC-CS only)
- OTSGs
- Furnaces

As mentioned, due to the larger request of auxiliary power for CO_2 capture, the GC-CS requires an additional natural gas fueled cogeneration unit. Instead, the GC-VS doesn't use this unit. The electricity production of the GC-VS can satisfy the demand of the processes. The last three facilities are identical to the one described in Chapter 4 and are not particularly complicated in comparison to the gasification based polygeneration plant. The gasification based polygeneration plant is divided into 5 main hierarchies:

- Coal selection and milling
- Gasifier island
- Syngas treatment
- Cogeneration
- Steam generation

The main sheet of the Aspen gasification based polygeneration plant model is shown in Figure 36. The inputs for the model are:

- Petcoke produced
- Electricity demand
- Sour produced gas production
- HP Steam required
- Hydrogen required
- Superheated steam required
- Saturated steam required
- Heat/fuel gas demand for furnaces
- Fuel gas production

All these quantities were defined and calculated in Chapter 2. The outputs of the model are:



Figure 36: Aspen model of the gasification based polygeneration plant

- Natural gas consumption
- Electricity export
- CO2 emissions

4.4 COAL SELECTION AND DECOMPOSITION MODEL

This model derives from the fact that there are some difficulties in defining a solid fuel such as petcoke.

The coal selection and decomposing model is shown in Figure 37.

Aspen Plus permits the definition of non-conventional streams for solid fuels. In order to define a non-conventional stream and its properties, a property model should be selected. The non-conventional stream 'coal' was created for the petcoke and the property method HCOALGEN was selected. This model requires as an input the proximate, ultimate and sulphur analysis. For the petcoke, it was decided to not use any model for the prediction of the lower heating value. Rather, it has been entered manually. The input values for the petcoke are the ones shown in Table 27 (composition) and Table 28 (LHV). A non-conventional stream for the ash ('ash') was also created. This stream in the proximate and ultimate analysis is solely composed from ash.

The gasifier reactor cannot handle non-conventional streams. Therefore, there is a necessity to convert the non-conventional stream 'coal' into a conventional stream. In order to do that, the block 'DCOMP' was used. The block 'DCOMP' is modeled with an RYield block. RYield models a reactor by specifying reaction yields of each component. The reactor is governed by a calculator block. This calculator block uses the moisture content in the proximate analysis (wet coal basis in Aspen) to convert the coal's ultimate analysis (dry coal basis in Aspen) to a wet coal basis ultimate analysis. This yield is what RYield uses to 'convert' the incoming mass into outgoing mass. The equations used in the calculator block are:

$$Factor = \frac{(100 - Moisture_{Proximate})}{100}$$
(4.1)

$$Water = \frac{Moisture_{Proximate}}{100}$$
(4.2)

Where $Moisture_{Proximate}$ is the % of moisture in the proximate analysis and *Factor* is a parameter to convert the dry ultimate analysis into wet ultimate analysis. Water is the mole fraction of water of the outlet steam of the 'DCOMP' unit. And for each component i of the ultimate analysis:

$$WETultimate_i = DRYultimate_i * Factor$$
(4.3)
Where $WETultimate_i$ is the component i in the wet ultimate analysis, while $DRYultimate_i$ refers to the component i in the dry ultimate analysis (Aspen input). The components of the wet ultimate analysis are defined as Aspen conventional components. The carbon and sulphur are associated with CSOLID components. The H2, N2, O2 and Cl2 are associated with MIXED components.

The Ash passes from the non-conventional stream 'coal' to the non-conventional stream 'ash'.

The outlet temperature of the block should be the same as the input temperature:

Tout = Tin

(4.4)

Since the moisture content of the fuel is very low, no drying unit is required. This unit is always included when commercial coal is used.

Before the gasifier, additional ash is added to the petcoke in a mixing unit. The amount of ash added is the same of the flyslag separated by the ceramic filter (Section 4.5).



Figure 37: Coal selection and decomposing model

The main reason for this operation is that the petcoke has a low content of ash, which is essential for the correct working conditions of the membrane wall (but also for refractory liners). Accordingly to Higman [44], it is essential to add ash when petcoke is gasified in slagging gasifiers with a membrane wall.

It has been assumed that the recirculation of the flyslag creates the correct working conditions for the membrane wall. If not, additional slag should be added or the petcoke should be mixed with high ash content coal.

The stream produced is then sent to the gasification model.

4.5 GASIFIER MODEL

The gasifier island has been modeled according to the general scheme of the Shell/Prenflo gasifier indicated by Higman [44]. Most of the operative parameters used for the Aspen model have been taken from the literature [44] [8].

The gasifier model is shown in Figure 38.

The gasifier has been modeled with an RGibbs reactor. The gasifier receives as an input the outlet temperature and the pressure drops. The streams entering the gasifier are steam, oxygen and nitrogen from the lock hoppers.

Since 100% of carbon conversion does not occur in the gasifier, a split unit before the reactor was introduced. The unconverted carbon bypasses the gasifier and is mixed with the syngas after the RGibbs unit. According to Higman [44], a value of carbon conversion of 99.5 % was taken.

There are three parameters that should be selected in order to produce the highest possible quality of syngas:

- Flowrate of oxygen
- Flowrate of steam
- Outlet temperature of the gasifier

One parameter that measures the 'quality' of the gasification is the cold gas efficiency (CGE):

$$CGE = \frac{\dot{m}_{sg} * LHV_{sg}}{\dot{m}_{fuel} * LHV_{fuel}}$$
(4.5)

Where \dot{m}_{sg} and LHV_{sg} are respectively the mass flow rate and the LHV of the syngas, while \dot{m}_{fuel} and LHV_{fuel} are the mass flow rate and LHV of the gasified fuel. In this simulation, the three parameters listed above vary in order to maximize the CGE. There are some constraints that should also be taken into account:

- The heat losses to the membrane wall have a fixed value
- The amount of CH₄ in the reaction should be minimized
- There is a CO₂ content in the syngas in the operative conditions

This problem can be easily solved with the optimization model analysis tool of Aspen Plus. The values for the oxygen and steam consumption are suggested by Higman [44]. The temperature cannot be lower than the ash fusion temperature for the correct operation of the membrane wall (see Table 28). The heat losses value for the membrane wall has been taken from [8]. The mole fraction values of CO_2 and CH_4 in the syngas have been taken from Higman [44]. The results of the optimization process are shown in Table 30.

The value of the CGE obtained, which is measured before the scrubber, is slightly lower than the values obtained with commercial coal (>80%). This is primarily due to the quality of the fuel.

The petcoke is hydrogen deficient and the syngas obtained is richer in CO and poorer in H_2 than the syngas generated from conventional coal. The composition of the syngas generated by conventional coal in a Shell gasifier is usually around one third H_2 and two thirds CO. In this case, the percentage of H_2 in the syngas is around 27%. Therefore, the heating value of the syngas and the CGE are lower. The membrane wall has been modeled as a steam generator that receives the heat fixed by the optimization and produces medium pressure steam. The pipes receive saturated steam at 42 bar and evaporate it. The amount of steam generated is regulated by a design spec block.

After the gasifier, a separator mixes the unconverted carbon and separates the coarse slag. This block simulates what occurs at the bottom of the Shell gasifier, where the coarse slag is collected and removed. According to Martelli [8], around 35 % of the input mineral matter exits the bottom of the gasifier.

After the separator a mixer simulates the syngas quench. Part of the cold syngas is recirculated by a blower.. The amount of syngas recirculated is regulated by a design spec block that fixes the quench temperature to 900 °C.

Parameter	Unit	Value	Result		
Variables					
Oxygen	kgO2/kgFuel	0.8-1.1	0.991		
Steam	kgSteam/kgFuel	0-0.36	0.196		
Temperature	°C	1480-1600	1480		
Constraints					
Heat Membrane Wall	${ m MW}/{\dot{m}_{fuel}}*LHV_{fuel}$	0.015	0.015		
Mole fraction CO2 Syngas	%	0.5-4	0.5		
Mole fraction CH4 Syngas	%	< 0.1	0.089		
Objective function					
CGE	%		75		

Table 3	80+ V	Variahles	ranges	hne	constraints	for	the o	ntimization	of the	Gasifier
Table S	JU.	v al lables	ranges a	anu	constraints	101	the o	pumization	or the	Gasmer

The syngas cooler is simulated as a simple cooler block with an outlet heat stream. The steam generation will be better explained in Section 4.7.

The flyslag is then separated into another separator block that simulates the candle filters. In that block all the ash is removed from the syngas. After the filter, a small part of the ash is disposed (5% bleed) and the rest is recirculated.

The input parameters of the gasifier are shown in Table 31.



Figure 38 : Gasifier Aspen Model

Parameter	Unit	Value	
Gasification pressure	bar	38.5	
Carbon conversion	%	99.5	
Oxygen inlet pressure	bar	46	
Oxygen inlet temperature	°C	100	
Oxygen purity	%	95	
Steam inlet temperature	°C	320	
Steam inlet pressure	bar	42	
Hp N2 into syngas/dried coal	Wt%	0.103	
N2 pressure	bar	68	
Heat to membrane wall	% of fuel	1.5	
	power	1.0	
Water membrane wall pipes pressure	bar	42	
Water membrane wall pipes inlet temperature	°C	250	
Water membrane wall pipes outlet temperature	°C	320	
Coarse slag percentage (%wt of total ash)	%	35	
Fly slag percentage (%wt of total ash)	%	65	
Syngas quench temperature	°C	900	
Flyslag bleed	%	5	
Syngas coolers outlet temperature	°C	250	
Syngas recycle (Result from Design spec)	%	49.25	

Table 31: Gasifier input parameters

4.6 SYNGAS TREATMENT MODEL

For the gasification based polygeneration plant, as was mentioned, a CO₂ venting scenario (VS) and a CO₂ capture scenarios (CS) are simulated.

In the VS the CO_2 produced is released in the atmosphere. In the capture scenarios a large part of the CO_2 contained in the syngas is separated, compressed and stored in extinguished reservoirs.

While the unit described in previous Sections is common, the syngas treatment is very different between the two scenarios. The flowsheet schemes for the VS and CS are shown respectively in Figure 39 and 44. The parameters used for the model are shown in Table 32.

4.6.1 Venting scenario (GC-VS)

The syngas treatment for the VS consists in several hierarchies. The main processes involved, in this order, are:

- Wet scrubbing
- COS hydrolysis
- Acid gas removal (H₂S only)

The syngas generated is then split into 2 different flows:

- Syngas used in gas turbines for cogeneration
- Syngas further treated for pure hydrogen generation

The last flow is sent to a water gas shift model where the syngas is transformed into a hydrogen rich flow. The syngas is then sent to a pressure swing adsorber (PSA) where hydrogen with a high level of purity and offgas is generated. The offgas generated is then used for the postfiring in the cogeneration system. The Aspen scheme of the syngas treatment in the VS is shown in Figure 40.

Wet Scrubbing

This unit has the goal of removing the last solids remaining after the candle filter. In most of the existing plants, the solids are washed out with water in this unit.

The scrubbing takes place below the dew point of the gas. The finest particles act as nuclei for condensation, thus ensuring the complete removal of solids.

In Aspen plus, there are many difficulties in modeling the solid removal. Moreover, in this model, all solids have been previously removed in the ceramic filter. However, a representation of the scrubber is not useless.

In fact, a large amount of water is injected into the scrubber to remove the solids. The scrubbing process changes the temperature of the syngas as well as its composition. Because of that, it is important to take account of this process and simulate it, even if the solid removal is not included. The scrubber model is shown in Figure 41

The scrubber is simulated as RadFrac column. RadFrac is a rigorous model for simulating all types of multistage vapor-liquid fractionation operations.

This unit was simulated with 5 stages, no reboiler and no condenser. The syngas enters at the bottom of the column (stage 5), while the water enters at the top (stage 1). The pressure selected for the process is 37 bar. The amount of water used for the scrubbing is equal to the flowrate of syngas. The water inlet temperature of the scrubber is 166 °C.



Figure 39: Flowsheet scheme for gasification based poligenerative plant in VS



Figure 40: Syngas treatment Aspen model, VS



Figure 41: Wet scrubber Aspen model

The RadFrac column works according to Henry's law. The Peng-Robinson model, which was used as the default property method for the syngas stream, does not allow Henry's law.

Because of that, the stream is switched to another property method that allows Henry's law. The ELECNRTL property method was selected.

After that, a Henry's component group was defined using the Henry Comps forms. After the scrubbing, a switch block turns back to the Peng-Robinson property method. The water outlet of the scrubber is then purified from the acid components and recycled to the scrubber. Since some water evaporates into the syngas, a make up of water is required. The recycled water, along with the make up, needs to be heated again to 166°C before being reintegrated into the column. The heat required is taken from cooling after the shift process of the hydrogen production.

The syngas exiting from the scrubber has a temperature of 148°C. All the parameters used for this unit are shown in Table 32.

COS hydrolysis

In the syngas produced by gasification, sulphur is not present only as H2S, but also as COS. While some sulphur removal washes (such as Rectisol) can remove COS along with H2S, amine washes do not remove COS. If the desulphurization has to be complete COS should be converted into H_2S before the AGR.

The COS can be selectively converted into H₂S through catalytic hydrolysis reaction:

 $COS + H_2O \rightarrow H_2S + CO_2$ $\Delta H_{298}^0 = -30 \text{ KJ/kmol}$

According to Higman [44], the optimum operating temperature is in the range of 150-200°C. The catalyst also promotes the hydrolysis of HCN.

The Aspen model of the COS hydrolisis is shown in Figure 42.

The syngas is preheated by the outlet flux of the hydrolysis reactor. For this heat exchanger, an approach difference of temperature of 25 K has been used.

The syngas is then heated to 200 °C with some of the heat from the syngas coolers. The hydrolysis reactor has been modeled as an RGibbs reactor where all the components are inert except the one involved in the COS hydrolysis reaction (Equation 4.6).

The syngas is then cooled to 38 °C and the water is condensed and removed. Some of the heat exchanged is recovered and used to preheat the sweet syngas, while some is lost in the process. All the parameters used for this unit are shown in Table 32.



Figure 42 : COS and HCN hydrolysis Aspen model

Acid Gas Removal (AGR)

After the COS hydrolysis there is the AGR unit. The SULFINOL-M was used as a process for the absorption of the H_2S . The separation of the H_2S has been done with a simple separator block.

The data for this block has been taken from [8].

The heat for the reboiling of the water is taken from the syngas coolers after the shift process of the hydrogen production.

The AGR model is shown in Figure 43. All the parameters used for this unit are shown in Table 32.

The mass of the water for the stripping has been calculated by a calculator block with the equation:

$$m_{water} = \frac{Heat_{stripping} * m_{H2S}}{\Delta H_{eva-7.5 \ bar}}$$
(4.6)



Figure 43: AGR Aspen model for VS

Where $Heat_{stripping}$ is the specific heat (kJ/kg) required for the stripping, \dot{m}_{H2S} is the mass flow rate of H2S and $\Delta H_{eva-7.5 \ bar}$ is the specific enthalpy for evaporation. $\Delta H_{eva-7.5 \ bar} = 2056.63 \ KJ/kg$ has been taken from the water properties tables of Spirax Sarco website [45].

The syngas for the Gas turbine is then preheated with some heat from the syngas coolers and used for electricity generation.

The syngas for the Hydrogen production is then sent to the WGS model.

Water Gas Shift (WGS)

For the shift reaction, the same two-stage configuration showed in Section 3.5 for the natural gas steam reforming was used. The catalysts used in this case are different from the ones used in the methane steam reforming process. The amount of CO in the syngas produced by gasification is much higher than the one from the steam reforming process. Furthermore, the catalysts used in Section 3.5 are not tolerant to sulphur, even in very minimal amounts.

The syngas feed of both shift reactors is at 250 °C. The Steam to CO molar ratio for the process is 2.5.

The heat from syngas cooling after the shift reactors is used to produce steam and to preheat water.

The shifted syngas is then sent to a PSA where pure hydrogen is produced. The PSA has been modeled as the one of Section 3.5.

The parameters used in the syngas treatment model are shown in Table 32.

4.6.2 Capture scenario (GC-CS)

The Syngas Treatment for the GC-CS itself consists in some hierarchies. The main processes involved, in this order, are:

- Wet scrubbing
- Water gas shift
- Acid Gas Removal (H2S and CO2)

The syngas generated is then split into 2 different flows:

- Syngas used in gas turbines for cogeneration
- Syngas further treated for pure hydrogen generation

The last flow is sent to a pressure swing adsorber (PSA) where hydrogen with a high level of purity and offgas is generated.

The offgas generated is then used for the postfiring in the cogeneration system. The Aspen scheme of the syngas treatment in the CS is shown in Figure 45.

Models

Since the design of most of the hierarchies used in the CS is the same of the ones used in the VS, their description will not be repeated.

Nevertheless, some considerations can be made:

- In the CS, the WGS involves all the syngas produced, not just a part of it (like in the VS). The WGS process requires a high amount of medium pressure superheated steam, which has to be produced in the ploygeneration plant. The amount of steam required is proportional to the syngas processed. Because of that, the need for steam in the CS is much higher than in the VS.
- The WGS process takes place before the AGR and in the presence of sulphur. This makes the use of sulphur-tolerant Co-Mo alumina catalysts absolutely mandatory.
- In the CS there is no need for a COS hydrolysis reactor. This is because the COS hydrolysis takes place in the WGS reactors, where the abundance of water and the thermodynamic conditions promote the COS hydrolysis reaction.
- The WGS converts almost all of the CO (around 98%) during the shift process. Therefore, after the CO2 removal, the syngas produced is mainly composed of H2 (94 %mol). The characteristics of the syngas produced in the two 'scenarios' are completely different. The syngas produced in the VS is mainly composed of CO (with around 25%mol of H2) and has a low LHV. The syngas produced in the CS, due to the high presence of H2, has a very high LHV.

After the shift, the syngas is cooled to the proper conditions for water condensation and acid gas removal.

The SELEXOL process was used for the absorption of the H2S and the CO2. The separation in this case has also been done with a simple separator block. The calculation for the mass of water required for the stripping has been done according to Equation 4.7. Although the simplified Aspen Plus scheme for the AGR is similar in both scenarios, the energy requirements involved in the process are very different. In fact, the CO2 absorption process requires much more heat and electricity than the simple separator of the H2S. After the AGR the syngas is preheated to around 60°C and sent to a separator block. All the parameters used for the units in the CS are shown in Table 32. Some of the syngas is then sent to the hydrogen production, while another part is sent to the cogeneration model.



Figure 44: Flowsheet scheme for the gasification based poligenerative plant in CS (with CO₂ capture)



Figure 45: Syngas treatment model for GC-CS

Parameter	Unit	Value			
Wet Scrubber					
Scrubber water inlet temperature	°C	166			
L/G ratio in Scrubber		0.25			
COS hydrolysis reactor					
COS hydrolysis reactor inlet temperature	°C	200			
Reactor heat duty	MW	0			
WGS					
Steam to CO ratio	mol steam/mol CO	2.5			
Steam temperature	°C	270			
High Temperature Shift inlet Temperature	°C	250			
HTS Heat Duty	MW	0			
HTS pressure Drops	bar	0.5			
Low Temperature Shift inlet Temperature	°C	250			
Pre Reformer Heat Duty	MW	0			
LTS pressure Drops	bar	0.5			
HTS/LTS reactor approach temperatures	°C	10			
Condenser Temperature	°C	38			
PSA inlet Temperature	°C	38			
PSA Hydrogen Split fraction	%	0.9			
PSA hydrogen Quality	%	1			
Sulfinol-M for removal o	fH2S				
LT heat for stripping	MJ per kg of stripped H2S	13.4			
CO co-absorbed	%	0.265			
H2 co-absorbed	%	0.268			
CO2 co-adsorbed	%	16			
Selexol for selective removal of CO2 & H2S					

LT heat for stripping	MJ per kg of stripped H2S	44.7
CO2 adsorbed	%	96.54
CO co-absorbed	%	0.44
H2 co-absorbed	%	0.553
Heat exchange parame	ters	
Syngas coolers & wet scrubber pressure drop	%	4
Heat exchangers pressure drops, gas side	%	0.05
Heat loss from heat exchangers	%	0.5
Syngas coolers: pinch point temp. diff. HT/LT coolers	К	50/20

4.7 STEAM GENERATION MODEL

In the gasification based poligenerative plant there is a certain production of steam. The steam is produced with the heat from the cooling of the syngas. The heat is available from these units:

- Membrane wall
- Syngas coolers
- HTS coolers
- LTS coolers

Furthermore, some units have a certain requirement for steam:

- Medium pressure steam for the gasification
- Medium pressure steam for the WGS
- Low pressure steam for the AGR stipping

The fact that the steam required from the gasification plant should be at a higher pressure than the syngas one (38.5 bar) prompts us to take 42 bar as a value for the medium pressure steam. This value of pressure is also optimal for the delayed coker, which demands steam at around 40 bar.

The system of heat exchangers is quite complex and is shown in Figure 46. Generally speaking, the LTS coolers preheat the water for medium pressure steam generation. They also produce hot water for the scrubber and low pressure steam for the AGR. The evaporation of the medium pressure steam is done mainly in the HTS coolers, the syngas coolers, and the membrane wall.

The evaporation of the low pressure steam required for the upgrading is done in the syngas coolers.

In the VS, the syngas coolers also produce some high pressure steam for the wells. However, in the CS, , no high pressure steam is produced from the syngas cooling. Furthermore, the superheating of the medium pressure steam takes place at the entrance of the OT-HRSG. This occurs because there is a much higher demand of steam from the WGS unit and there is no more heat available for the superheating. The parameters used for the Aspen model are shown in Table 32.

4.8 COGENERATION MODEL

4.8.1 Syngas fueled gas turbines performances

The syngas produced is then sent to the cogeneration model. As mentioned, the composition of the syngas is very different in the two cases. The syngas composition after the AGR is shown in Table 33.

Component	VS	CS
H2	27.98	94.15
СО	69.83	1.35
CO_2	0.02	2.34
AR	1.07	1.05
H ₂ O	0.01	0.01
CH ₄	0.08	0.08
N ₂	1.01	1.02

Table 33: Composition (%mol) of the syngas

A decision was made to maintain the same gas turbine for the GC, the 47.5 MW Siemens SGT-800 [32] used in the reference case.

This decision was made for two reasons. First of all, the comparison between the different cases should be 'fair'. There are a lot of large size machines successfully working with syngas. Nonetheless, these units are more efficient than the small size turbine selected for the reference case. For this reason, the GC will be advantaged compared to the RC. Secondly, the oil sands companies prefer to use small/medium size gas turbines. Unfortunately, commercial gas turbines are designed for natural gas and their use with syngas leads to some issues.



Figure 46: Steam generation model (VS)

The most important concern is the mitigation of NOx emissions, which becomes critical due to the very high H2 flame temperature.

Accordingly to Gazzani [46], two different methods can be proposed to control NO_X emissions from gas turbines:

- Premixed lean combustor
- Diffusive flame dilution with inert species (steam, water or nitrogen)

The second technology is mature and fully developed. In fact, throughout a saturator and/or the addition of the nitrogen available from the Air Separation Unit (ASU) a dilution of the syngas is possible, which leads to a lower flame temperature and lower NOx emissions. However, the addition of inert gases for diffusive combustion is conducive to a penalty concerning efficiency. Furthermore, this technology can require even more modifications on the gas turbine design than the one required by simple syngas use. In fact, the addition of inerts leads to an increment of gases at the turbine inlet turbine which cause off-design operation problems.. If water is added to the fuel, then the heat transfer rate on the turbine blades will be more likely to cause problems on the blades cooling. The premixed lean combustors are not available on the market yet. The main challenge in

the development of this technology is that, due to the high reactivity of the hydrogen, it is very difficult to premix air and hydrogen with acceptable pressure drops.

Nevertheless, there is significant investigation on this matter, with discrete results. [47] [48]. Chen [48] asserts that Dry Low NOx (DLN) combustors with swirl premixers operating in pilot scale will soon be available on a large scale for syngas fueled gas turbines.

Because of these reasons, a DLN combustor design was selected for the syngas-fueled SIEMENS SGT-800 gas turbine.

The performances of the SGT-800 machine were simulated with the software GT-PRO. The composition of the syngas shown in Table 33 has been used as fuel input for the GT-PRO simulation. The parameters used for the corrected site conditions have also been inserted as inputs for both VS and CS, shown in Section 3.3.1. The results of these simulations are shown in Table 34

Table 34: Performances of the syngas fueled 2008 SIEMENS SGT-800 in the
Corrected site conditions simulated with GTPRO

Parameter	Unit	Natural Gas	VS	CS
Power	MW	48.93	50.17	52.25
Efficiency	%	37.36	37.5	38.36
Air mass flow rate	kg/s	134.35	134.31	134.3

Fuel mass flow rate	Kg/s	2.65	10.61	2.37
Flue gas mass flow rate	kg/s	137	144.92	136.7
TIT	°C	1292.9	1278.3	1298
Turbine outlet (TOT)	°C	540.8	535.5	538.62

Furthermore, it was assumed that the shaft and the generator of the turbine have a power limit superior to the one produced by the turbine.

4.8.2 Cogeneration unit model

The cogeneration model in Aspen plus and its parameters are identical to the one designed in the reference case in Section 3.3.2.

The turbine, as in the reference case, has been designed with an equivalent model that produces the output of the GT-PRO simulation (Table 34).

The number of turbines installed has been selected with these equations:

$$m_{sg-cogen} = m_{sg-prod} - m_{sg-h2prod}$$

$$\tag{4.7}$$

$$NUMGT = INTINF(\frac{m_{sg-cogen}}{m_{sg-1turb}})$$
(4.8)

$$m_{sg-turb} = m_{sg-1turb} * NUMGT \tag{4.9}$$

$$m_{sg-pfire} = m_{sg-cog} - m_{sg-turb}$$

$$(4.10)$$

Where $m_{sg-prod}$ is the total mass flowrate of sweet syngas produced after the AGR, $m_{sg-h2prod}$ is the mass flow rate of syngas for the hydrogen production, $m_{sg-cogen}$ is syngas mass flow rate to the cogeneration unit. NUMGT indicates the number of gas turbines installed $m_{sg-1turb}$ represent the amount of syngas used in one turbine, $m_{sg-turb}$ is the total mass flow rate to gas turbines and $m_{sg-pftre}$ is the syngas burned for postfiring. A maximum temperature of 750 °C has been selected for the postfire, as in Section 3.3.2. Since the amount of syngas allocated for the postfiring is not sufficient to reach the desired temperature (750 °C), a small amount of natural gas is used. The composition of the natural gas used is equal to the one used for the reference case (Table 18). The results of the equations 4.6-4.9 are shown in Table 35.

Table 35: Syngas use in power island and hydrogen production

Parameter	Unit	VS	CS
$\dot{m_{sg-prod}}$	kg/s	102.36	20.16

$\dot{m_{sg-h2prod}}$	kg/s	31.73	6.26
$m_{sg-cogen}$	kg/s	70.63	13.91
GT nominal net power	MW	50.17	52.25
$m_{sg-1turb}$	kg/s	10.61	2.37
NUMGT		6.00	5.00
$\dot{m_{sg-turb}}$	kg/s	63.66	11.85
m _{sg-pfire}	kg/s	6.97	2.06

4.9 GASIFICATION BASED POLIGENERATIVE PLANT PERFORMANCE

In this Section, the performances of the gasification based poligenerative plant model are analyzed. The performances analyzed in this section are just referred to the gasification based poligenerative plant, which is a part of the gasification case. Instead, the results of the overall GC are studied in Section 4.10.

In Table 36 the plant power production and consumption are shown. The parameters used to calculate the consumption of the auxiliary units are taken from Martelli's work [8]. Generally speaking, the ASU power consumption is proportional to the flow rate of oxygen (2.482 MJ/kg O2). The coal handling consumption is proportional to the amount of coal used as a feedstock for the gasifier instead (1% of thermal power in).

The CO2 drying and compression power consumption is proportional to the CO2 captured (222.7 kJ/kgCO2)

As is evident in the results, the electricity consumption of the ASU is, by far, the largest of the auxiliary units.

Parameter	Unit	VS	CS
ASU, O ₂ & N ₂ compressors	MW	124.60	124.60
Coal handling	MW	17.81	17.81
AGR, Claus, SCOT units	MW	0.19	18.11
CO2 drying and compression	MW	0	32.26
Total auxiliary power	MW	142.6	192.77
GTs net power	MW	301.02	261.25
Net electric power	MW	158.42	68.48

Table 36: Plant power performances, with breakdown of power consumption by unit

As a result, the auxiliary consumption in the CS is around 35% superior to that of the VS. Because of that, the net electric power in the CS is much lower.

The results for the steam generation are shown in Table 37.

As was mentioned before, the steam demands of the WGS are much larger in the CS than in the VS. Because of this reason, the CS produces around 25 % less high pressure steam. The overall performances of the gasification based poligenerative plant are shown in Table 38. As was mentioned before, some natural gas has been used in the postfiring system in order to heat the flue gases to 750 °C.

Parameter	Unit	VS	CS
HP-MP-LP pressures	bar	100-42-20	100-42-20
LP steam Produced	kg/s	16.7	16.7
LP steam from SG coolers	kg/s	16.7	16.7
MP steam Produced	kg/s	73.88	170.86
Mp steam into gasifier	kg/s	9.94	9.94
MP steam bleed into WGS	kg/s	47.84	144.81
MP steam to upgrading	kg/s	16.11	16.11
HP steam produced for SAGD extraction	kg/s	240.86	182.62
HP steam from SG coolers	kg/s	38.13	0
HP steam from OT-HRSG	kg/s	202.72	182.62

Table 37: Steam production performances, with breakdown of steam consumption

1 'Capture 60' scenario is identical to CS, with an input of petcoke of 60 kg/s instead of 50.66 kg/s

The efficiency calculated in Table 38 are referred to this equations:

$$\eta_{net} = \frac{\dot{m}_{H2} * LHV_{H2} + \dot{m}_{LPS} * \Delta H_{MPS} + \dot{m}_{MPS} * \Delta H_{MPS} + \dot{m}_{HPS} * \Delta H_{HPS} + PWR_{net}}{\dot{m}_{NG} * LHV_{NG} + \dot{m}_{PCK} * LHV_{PCK}}$$
(4.11)

Where :

 $\dot{m}_{\rm H2}$, $LHV_{\rm H2} = Mass$ Flow rate and LHV of hydrogen

 \dot{m}_{LPS} , $\Delta H_{LPS} = Mass$ flow rate and specific variation of enthalpy of the LP steam

produced (Sat@20bar)

 \dot{m}_{MPS} , $\Delta H_{MPS} = Mass$ flow rate and specific variation of enthalpy of the LP steam produced (42 bar, 500 °C)

 \dot{m}_{HPS} , $\Delta H_{HPS} = Mass$ flow rate and specific variation of enthalpy of the HP steam

produced (Sat@100bar)

 \dot{m}_{PCK} , LHV_{PCK} = Mass Flow rate and LHV of the gasified petcoke

 \dot{m}_{NG} , LHV_{NG} = Mass Flow rate and LHV of Natural Gas

 $PWR_{net} = Electricity produced (Net from auxiliaries consumption)$

 $\eta_{net} = \text{Net efficiency of the gasification based poligenerative plant}$

The results of Table 38 confirm the very high performances of this plant for this application. In particular, the VS has resulted in satisfactory output of both net power (158.42 MW) and steam (616.2 MW).

The energy penalty for the CO2 capture is around 10 %, which is a typical value for this application. Nevertheless, the net efficiency has an incredibly high value for a plant with CO2 capture.

However, in the CS, the net electricity output turns out to be too low to satisfy the demand of electricity by the processes, even for the low energy scenario. Due to this problem, it is mandatory to install additional natural gas-fueled gas turbines.

Parameter	Unit	VS	CS
Petcoke in	kg/s	50.66	50.66
	MW	1781.05	1781.05
Natural gas in	kg/s	2.07	0.67
	MW	101.74	32.93
H2 produced	kg/s	2.65	2.65
	MW	317.89	317.89
LPS produced	kg/s	16.7	16.7
	MW	32.73	32.73
MPS produced	kg/s	16.11	16.11
	MW	55.42	55.42
HPS produced	kg/s	240.86	182.62

Table 38: Gasification plant overall performances and efficiency

	MW	528.06	400.88
Overall steam	MW	616.2	456.3
Gross power	MW	301.02	261.25
Net power	MW	158.42	68.48
Steam/Netpower Ratio	MW _{steam} /MW _{power}	3.89	6.67
Net efficiency	%	58	48.26

In Table 39 the CO2 emissions of the gasification plant are displayed.

The VS, despite its high efficiency, turns out to be a very high producer of CO2. The CS can efficiently capture 93.3 % of the CO2, which is a very good result.

Parameter	Unit	VS	CS
CO2 produced	kg/s	158.5	155.3
CO2 captured	kg/s	0	144.84
CO2 vented	kg/s	158.5	10.45
CO2 capture level	%	0	93.3

Table 39: CO2 emissions of the gasification plant

4.10 RESULTS

In this section, the main results of the model for the gasification case (GC) are shown. In the previous section, only the performances of the gasification plant were shown, without any integration within the SAGD and upgrading processes. In this section, the gasification based polygeneration plant is simulated along with the unit described in Section 4.1, in order to fully satisfy the energy demand calculated in Chapter 3.

Analogously to Section 3.8, the energy requirements of the various units were calculated. After that, a net energy analysis was made and the CO_2 emissions were calculated. In the end, these results have been compared to the results of the reference case.

4.10.1 Energy consumption in the GC model

In the GC model the energy is provided to the energy facilities with both solid and gaseous fuels. The solid fuel used is the petcoke (PCK), while the gaseous fuels used in the SCO Life Cycle (LC) are natural gas (NG), produced gas from wells (PG), and fuel gas (FG) from coker.

A specific consumption of fuel was related to every unit. The attribution of fuel consumption to the gasification unit was not so simple. In fact, this unit produces energy

streams for different purposes. A decision was made to divide the energy streams into two major groups:

- Electricity production
- Steam generation and hydrogen production

It was decided that the natural gas consumption for electricity generation is the syngas stream used in the simple cycle of the gas turbine. The steam generation and hydrogen production is proportional to the syngas processed in the hydrogen production process. The offgas produced in this process is used as a fuel for steam generation. The calculations have been done for a high energy scenario (HES) and a low energy scenario (LES). The GC was simulated both in the VS and in the CS. The results of the two different simulations with Aspen Plus are shown in Tables 40 and 41. The results show an increase in energy consumption between the LES and HTS (+35%), especially due to the highest consumption of natural gas in OTSGs.

4.10.2 NEA

The NEA has been done with the same methodology and the same equations used in Section 3.8.2. The results of the NEA are shown in Table 42.

The NER, as a consequence of the increment in the energy requirements, increased from the LES to the HES and from the VS to the CS.

However, the values of NEER are very high in both cases. In the VS, the values of NEER are probably close to that of conventional crude. Generally speaking, it means that for every MJ that is externally entered into the SCO process, 9.19-26 MJ of energy are produced. Using an expression of Brandt and Dale [39], with these high values of NEER, there is a big growth in energy supply to society.

The values of NEER of the CS are lower. This is caused by the additional cogeneration unit, which is using some natural gas. However, the value of the NEER is still high also for the CS.

Block	DN NG	NG NG	PG	FG	PCK	PCK	Energy	Energy
		-(can)						
	kg/s	kg/s	kg/s	kg/s	kg/s	kg/s	MW	MW
GASIFIER	2.65	2.65	0.00	0.00	50.66	50.66	1781.05	1781.05
ELECTRICITY	0.00	0.00	0.00	0.00	34.96	34.96	1228.95	1228.95
H2 & SG	2.65	2.65	0.00	0.00	15.70	15.70	682.35	682.35
ADDITIONAL COGENERATION	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OTSGs	4.75	18.44	3.61	9.42	0.00	0.00	754.67	1427.64
FURNACES	0.00	0.00	0.00	13.30	0.00	00.0	637.72	637.72
TOT	7.40	21.09	3.61	22.83	50.66	50.66	3303.70	3976.67
1 LES refers to Low Energy Scenario : iS	OR=2 and EOR	=7.5						
2 HES refers to High Energy Scenario: iS	OR=3 and EOR	=14						

Table 40: Energy consumption in VS

Dicol	Ŋ	ŊŊ	Ç,	C A	PCK	PCK	Energy	Energy	
DIUCK	$(LES)^{1}$	$(HES)^2$	2	LC.	(LES)	(HES)	(LES)	(HES)	
	kg/s	kg/s	kg/s	kg/s	kg/s	kg/s	MW	MM	
GASIFIER	0.67	0.67	0.00	0.00	50.66	50.66	1813.99	1813.99	
ELECTRICITY	0.00	0.00	0.00	0.00	34.96	34.96	1229.09	1229.09	
H2 & SG	0.67	0.67	0.00	0.00	15.70	15.70	584.90	584.90	
ADDITIONAL COGENERATION	6.70	6.70	0.00	0.00	0.00	0.00	329.32	329.32	
OTSGs	3.83	17.52	3.61	9.42	0.00	0.00	709.47	1382.35	
FURNACES	0.00	0.00	0.00	13.30	0.00	0.00	632.28	632.28	
TOT	11.20	24.89	3.61	22.72	50.66	50.66	3485.05	4157.93	
1 LES refers to Low Energy Scenario : iS	OR=2 and EOR	=7.5							
2 HES refers to High Energy Scenario : is	SOR=3 and EOR	1=14							

Table 41: Energy consumption in CS

Parameter	Unit	LES VS	HES VS	LES CS	HES CS
SCO Production	kg/s	204.24	204.24	204.24	204.24
	MW	9505.47	9505.47	9505.47	9505.47
Fuel gas Export	kg/s	0.00	0.00	0.00	0.00
	MW	0.00	0.00	0.00	0.00
Electricity Export	MW	62.61	21.99	70.88	30.25
Electricity Export in primary energy ¹	MW	156.525	54.97	177.2	75.62
Petcoke consumption	kg/s	50.66	50.66	50.66	50.66
	MW	1781.05	1781.05	1781.05	1781.05
Natural Gas Consumption	kg/s	7.40	21.09	11.20	24.89
	MW	363.79	1036.76	550.5	1223.38
Produced Gas Consumption	Kg/s	3.61	3.61	3.61	3.61
	MW	73.36	73.36	73.36	73.36
Fuel Gas Consumption	Kg/s	22.72	22.72	22.72	22.72
	MW	1098.84	1098.84	1098.84	1098.84
NER	GJ _{out} /GJ _{in}	2.88	2.39	2.76	2.3
NEER	GJ _{out} /GJ _{in}	26.30	9.19	17.4	7.79

 Table 42: Energy streams and ERRs of SCO production for the GC

1 An efficiency of 0.4 has been taken for Alberta's electric grid

4.10.3 CO₂ Emissions

The CO_2 emissions of the gasifier plant in VS and CS are shown in Table 43. The CO_2 capture in the gasification plant turns out to be effective not just in the gasifier performances, which have been shown in Section 4.9, but also in the integration into the process. The CS reduces the CO_2 emissions related to the SCO lifecycle to about 50% of the one of the VS.

Block	VS LES	VS HES	CS LES	CS LES
GASIFIER	158.5 (16.4)	158.5 (16.4)	10.4 (1.1)	10.4 (1.1)
ELECTRICITY	94.2 (9.7)	94.2 (9.8)	5.2 (0.5)	5.2 (0.5)

Table 43: CO2 Emissions in kg/s (g/MJ_{sco}) for the GC

H2 & SG	64.2 (6.6)	64.3 (6.66)	5.2 (0.5)	5.2 (0.5)
ADDITIONAL COGENERATION	0.0 (0.0)	0.0 (0.0)	18.3 (1.9)	18.3 (1.9)
OTSGs	46.4 (4.8)	83.7 (8.7)	43.9 (4.5)	81.2 (8.4)
FURNACES	39.0 (4.0)	39.0 (4.0)	39.0 (4.0)	39.0 (4.0)
CO2 AVOIDED	13.0 (1.3)	4.6 (0.5)	14.8 (1.5)	6.3 (0.6)
TOTLC	230.89 (23.94)	276.65 (28.69)	97.2 (10.08)	143.00 (14.83)

4.10.4 Gasification case (GC) Vs reference case (RC)

In this section, the results obtained for the GC and RC are compared. The results of the GC and the RC are shown in Table 44. The comparison between the GC and RC is shown in Table 45. For each parameter considered, the mean value between the LES and HES was taken.

Parameter	Unit	RC	GC-VS ¹	GC-CS ²
Power consumption (NG + FG +PG+ PCK)	MW	2974.24	3640.19	3826.85
NG consumption	MW	2203.33	700.28	886.94
FG + PG consumption	MW	770.91	1158.86	1158.86
PCK consumption	MW	0.00	1781.05	1781.05
Dependence on NG	%	74	19	23
NER ³	GJ_{out}/GJ_{in}	3,46	2,64	2,49
NEER ⁴	GJ _{out} /GJ _{in}	4.65	17.75	12.60
CO ₂ emissions	kg/s	168,84	253,77	120,12
	g/MJ _{SCO}	17,53	26,05	12.46

 Table 44 :Results of the GC and the RC

1 Venting scenario

2 Capture scenario

3 Net energy ratio in primary energy

4 Net external energy ratio in primary energy

Table 45: Comparison of the GCs with the RC

Parameter	GC-VS	GC-CS
Power consumption	+ 22,39 %	+ 28,49%
NG consumption	- 68,22%	- 59,75%
Dependence on NG	- 74,03%	- 68,67%

NER	- 23,84%	- 28,03%
NEER	+ 281,61%	+ 170,86%
CO ₂ emissions	+ 48,62%	- 28,93%

1 Compared to the RC

The energy consumption of the GC is higher than the one of the RC (+22.39% and +28.49%, respectively for the VS and the CS) .However, this parameter only refers to the amount of energy consumed, without any distinction on the fuel used. It is evident that using 1 MJ of natural gas is different than using one MJ of petroleum coke.

The RC relies entirely on natural gas, which is the finest fuel resource in commerce. All the technologies considered in the RC have a very high efficiency, mainly because of the quality of the fuel. Instead, the GC produces most of the energy with petroleum coke. This resource is usually stockpiled and is worthless because of the difficulties associated with its use. Thus, the GC offers the possibility to use, on a large scale, a resource as dirty and useless as petroleum coke with a very respectable efficiency.

The NER provides the same indication of the energy consumption. It is clear that with the gasification there is an overall larger use of energy, because of the lower efficiency of the processes. However, the extra energy comes from a waste product that is otherwise unusable.

For both the RC and GC, the natural gas is the only fuel 'imported' on the plant and used in the energy facilities. The GC, thanks to the contribution of the petcoke, can significantly reduce the natural gas consumption in both VS and CS. The result is an overall dependency on natural gas of 19% and 23% for the VS and CS, respectively.

The parameter that most highlights the performance of the GC is without any doubt the NEER. In fact, this parameter only considers the 'external' fuel consumption in the calculations. The petcoke and offgas produced in the upgraders are not considered as 'external' fuels because they were originally within the bitumen extracted from the subsoil. The values of NEER for the GC are 17.75 and 12.6 respectively for the VS and CS. These values are much higher than the ones obtained in the RC (4.65).

In simple terms, for each GJ of external energy introduced into the oil sands processes, we produce 12.6-17.75 GJ of primary energy. The increase of the value between the RC and GC is impressive (+281.61 % and + 170,86% for VS and CS, respectively).

Despite the undeniable advantages mentioned, the CO_2 emissions of the GC are much larger than the ones of the RC. The main reason is that petcoke is essentially fixed carbon. Due to the very low content of hydrogen, this fuel generates more CO_2 than practically all the commercial fuels. The natural gas, due to the high H to C ratio in the molecule, is the hydrocarbon that produces by far less CO_2 .

Therefore, the VS of the GC produces around 50 % more CO2 than the GC, which is an enormous amount. In a whole year, the VS of the GC would vent about 2.5 million more tons of CO_2 than the RC.

However, the CS of the GC, through the CCS, permits a considerable reduction $inCO_2$ emissions The results are a decrease of around 30% of the emissions of the RC, which means, over a year, around 1.5 million of tons of CO_2 .

CHAPTER 5: Conclusions

This work was focused on SAGD extraction of bitumen from oil sands industry and upgrading to synthetic crude oil.

In particular, the energy consumption and the related emissions of two technologies were evaluated:

- Current technology, based on natural gas (reference case)
- Gasification of petroleum coke (gasification case), in venting and capture scenario

Both the reference and gasification cases were modeled with the software Aspen Plus from Aspentech. The results obtained for the reference case were similar to the one of other works done on this purpose. For this reason, the model can be considered reliable. Particularly, the reference case provides a closer range for the direct CO_2 emissions related to the upgrading than the other works in the literature. This result was obtained through the use of some experimental correlations for the calculation of the upgrading demand. We obtained a range of 15.48-19.57 gCO₂/MJ_{SCO} for the reference case.

In addition, a net energy analysis was performed. The result of a NEA is usually an energy return ratio, a parameter which compares the amount of primary energy consumed in exploitation of an energy resource to the amount of valuable primary energy provided to society.

Two energy return ratios were obtained: The net energy ratio considers the energy consumption to get a resource and is proportional to the total energy input . The net external energy ratio on the other hand , considers just the external primary energy used for a certain process. The reference case resulted in small values of energy return ratios. Values of 3.02-3.9 and 3.85-5.42 GJ_{out}/GJ_{in} were determined for the net energy ratio and the net external energy ratio respectively. These values are very low compared to the ones associated with conventional light crude (15-30 GJ_{out}/GJ_{in}).

The gasifier case produced very good results, even better than the expected one. There are not particular problems in adapting entrained bed gasifiers to petcoke use (except for the low content in ash). However, the particular poligenerative application considered results to be very effective. Part of the syngas was converted to pure hydrogen for refinery use, while the remaining was used to produce power. Thanks to the syngas coolers and to the posfired OT-HRSG, a large amount of steam was generated throughout the process. The gasification plant therefore, results to have a steam/power ratio of 3.09 and 4.09 for the VS and the C60S respectively. This value of the steam/power ratio compared to the value of 1.65 of cogenerations systems (with postfiring), seems to be better suited to the demand (13.6-13.99 MW_{steam}/MW_{power}).

The gasification based polygeneration plant results have a value of efficiency of 58% for the venting scenario and 48.6% for capture scenario. This results are very high compared to the common application of gasification plants. The polygeneration plant also offers very

good performances in the oil sands energy infrastructure. In both venting and capture scenarios, the gasification based polygeneration plant produce all the hydrogen and steam for the refinery. In the venting scenario, all the electricity for the processes can be produced with the syngas. In the capture scenario instead, an additional natural gas cogeneration unit is required in order to produce all the electricity for the processes. In the polygeneration plant, around 22-37% (depending on the energy scenario) of the steam required from the wells is produced. The rest of the steam can be easily integrated through OTSGs (and cogeneration in the capture scenario) using both the produced gas and the natural gas.

As a result, the dependence on natural gas is reduced from 74% in the reference case to 19-23% for the venting and capture scenarios of the gasification case.

Since the overall efficiency of the gasification case is lower than the one of the reference case, the energy consumption increase with respect to the reference case (22-28.5%). However, the energy source is much less valuable and this increment doesn't constitute any problem. On the contrary, the reduction in natural gas use increased by far the value of the net external energy ratio.

With the gasification case, we can obtain values from 9-26.3, which are very similar to the one obtained by conventional light crude. In simple terms, for each GJ of external primary energy introduced into the oil sands processes, 9-26.3 GJ of primary energy are produced. The energy used to extract the bitumen and to upgrade it to SCO is provided in large part from the bitumen itself, by the use of its main waste product (the petcoke). In the GC, every part of the bitumen extracted from the subsoil finds its proper application. This efficient conversion of the bitumen seems to be much more sustainable in the long term than the large input of external natural gas.

However, gasification case in venting scenario produces much more CO2 emissions. The main reason is that the petcoke is essentially fixed carbon. Due to the very low content of hydrogen, this fuel generates more CO_2 than practically all the commercial fuels. The natural gas instead, due to the high H to C ratio in the molecule, is the hydrocarbon that produces by far less CO_2 .

The venting scenario of the gasification case therefore, results in producing around 50 % more CO2 than the reference case, which is an enormous amount. In a whole year, the venting scenario of the GC would vent around 2.5 millions of tons of CO₂ more than the reference case. These number are unacceptable in the current global scenario, especially in a CO₂ constrained industry as Alberta's oil sands.

However, gasification offers some of the least costly methods for large scale CCS. The capture scenario decrease of the emissions by around 30%, which means, over an year, around 1.5 million of tons of CO_2 .

This reduction in the energy intensity is much higher than the one currently required by the government (12%) and can be therefore implemented in a long term horizon. Additionally, gasification of petcoke produces very low emissions of SO_2 thanks to the

very efficient removal of H₂S from the syngas.

From an economic point of view, however, this solution is not competitive yet. Gasification is very capital intensive. Moreover, despite the fact that Canada hosts one of the five CCS plant in operation in the world and is strongly investing in this technology, CCS is still very expensive.

In this particular moment, natural gas tends to be very cheap in North America and no resources can compete with it, especially from an environmental point of view. Moreover, since the price of the crude has sharply fallen down, the profits of the oil sands industries have been reduced.

Petcoke gasification with CO_2 capture would be an energetically and environmentally sustainable solution which would allow efficiently disposal of petcoke, while decreasing the natural gas consumption as well as the CO_2 emissions related to the extraction of Oil Sands.

Possible future developments

This work considered only the possibility of petcoke gasification from a technological point of view. No economical analysis were performed in this study. The final evaluation of this solution should pass through a feasibility analysis.

A future work can be the comparison between the gasification case and the reference case, from an economic point of view.

Moreover, petroleum coke from delayed coking is not the only resource that can be gasified in a Shell gasifier. Some other refinery waste products are generated in the oil sands industry (residues from de-asphalting, fluid coking ecc). The study of this processes combined with the gasification of these by-products can be compared with the results of this work.

In the end, due to the abundance of biomass in Alberta, co-gasification of petcoke and biomass can be performed. With this solution, CO2 emissions can be reduced further.

Bibliography

1. Alberta Oil sands Industry. Quarterly update. Spring 2015.

2. EIA. [Online] http://www.eia.gov/countries/index.cfm?view=production.

 Life Cycle Greenhouse Gas Emissions of Current Oil Sands Technologies: GHOST Model Development and Illustrative Application. Charpentier, Kofoworola, Bergerson, MacLean. 45, 2011, Enviromental science and technology, pp. 9393-9404.

4. McCullogh, Raynolds, Wong. Carbon Neutral 2020 A Leadership Opportunity in Canada's Oil Sands. October 2006.

5. State and trends of carbon pricing 2014. group, World bank. Washinton DC : s.n., May 2014.

6. *Petroleum coke as energy source: a critical evaluation*. **Pinelli.** 1, 2003, La rivista dei combustibili, Vol. 57.

7. *Gasification of Oil sands coke : Review.* **Furimsky.** 56, 1998, Fuel processing technology, pp. 263-290.

8. Shell coal IGCCS with carbon capture: Conventional gas quench vs. innovative configurations. Martelli, Kreutz, Carbo, Consonni, Jansen. 88, 2011, Applied Energy, pp. 3978-3989.

9. Huc, Alain-Yves. Heavy Crude Oil. From geology to upgrading. 2011.

10. Cenovus Energy. Foster Creek thermal project phase J expansion. Volume 1, Ch 4.

11. *Aquathermolysis and Sources of Produced Gases in SAGD.* **Thimm.** 10-12 June 2014. SPE Heavy Oil Conference Canada.

12. Jacob Consultancy. SAGD energy efficiency study. September 2009.

13. Cenovus Energy. Foster Creek in-situ oilsands scheme (8623). 2013.

14. General Electric. [Online] http://www.gewater.com/zero-liquid-discharge-zld.html.

15. *New SAGD technologies show promise in reducing enviromental impact of Oil Sands production.* Lightbown, Vicki. 2, : s.n., Oil, gas, and mining, Vol. 1, pp. 1-12.

16. Cenovus Energy. Foster Creek thermal project phase J expansion. Volume 1, Ch 6.

17. **Maddocks, Conacher, Dixon.** *Conversion of Suncor's South Rosevearfacility t o Acid gas injection.* 2008.

18. Meyers. Handbook of Synfuels Technology. 1986.
19. *Modeling the energy demands and the Greenhouse Gas emissions of Canadian oil sands industry.* **Ordorica Garcia, Croiset, Douglas, Elkamel.** 21, 2007, Energy and fuels, pp. 2098-2111.

20. Gary, Handwerk. Petroleum Refining Technology and Economics. 1994.

21. **AER.** [Online] http://www.aer.ca/data-and-publications/activity-and-data/in-situ-performance-presentations.

22. Artificial lift-A major unresolved issue for SAGD. Kisman. 8, August 2003, Journal of Canadian petroleum technology, Vol. 42.

23. Cenovus Energy. Cenovus Christina Lake In-situ Oil sands scheme (8591). 2013.

24. —. Foster Creek thermal project phase J expansion. Volume 1, Appendix F.

25. COSIA Challenge. Fouling resistant OTSG. [Online] http://www.cosia.ca/challenges.

26. Cud Baird, HPI consultants. Petroleum refining process correlations. 1987.

27. Maples. Petroleum refining process economics. 1993.

28. *Processing oil sands bitumen is Syncrude's R&D focus,*. **Yui, Chung, Keng.** April 23, 2001, Oil & Gas Journal, pp. 46-52.

29. AspenTech. [Online] http://www.aspentech.com/products/aspen-plus.aspx.

30. **National Energy Board.** [Online] https://www.neb-one.gc.ca/nrg/tl/cnvrsntbl/cnvrsntbl-eng.html.

31. **Union Gas.** [Online] https://www.uniongas.com/about-us/about-natural-gas/chemical-composition-of-natural-gas.

32. **Siemens.** [Online] http://www.energy.siemens.com/nl/en/fossil-power-generation/gas-turbines/sgt-800.htm#content=Description.

33. Thermoflow. [Online] http://www.thermoflow.com/combinedcycle_GTP.html.

34. *Methane steam reforming, methanation and water-gas shift: I. Intrinsic kinetics. AIChE Journal 1989; 35:88-96.* **Xu, Froment.** 1, January 1989, AIChE Journal, Vol. 35, pp. 88-96.

35. *Balancing Hydrogen Demand and Production : Optimising the Lifeblood of a Refinery.* **Bressan, Luigi.** Milan : s.n., 12-14 June 2012. IRPGC 2012.

36. Water Gas Shift Catalysis. Ratnasamy, Wagner. 3, 2009, Catalysts Review, Vol. 5, pp. 325-440.

37. Simulation and optimization of an industrial psa unit. Barg, Ferreira, Trierweiler, Secchi. 4,2000, Brazilian journal of chemical engineering, Vol. 17, pp. 793-807.

38. **Herendeen.** Net Energy Analysis: Concepts and Methods. *Encyclopedia of energy*. Vol. 4, pp. 283-289.

39. A General Mathematical Framework for Calculating Systems-Scale Efficiency of Energy Extraction and Conversion: Energy Return on Investment (EROI) and Other Energy Return Ratios. **Brandt, Dale.** 4, 2011, Energies, pp. 1211-1245.

40. Alberta Enviromental Climate Change Secretariat. *Technical Guidance for Completing Specified Gas Compliance Reports.* s.l. : Edmonton, Alberta T5J1G4, February 2011.

41. *The energy efficiency of oil sands extraction: Energy return ratios from 1970 to 2010.* **Brand, Englader, Bharadwaj.** 55, 2013, Energy, pp. 693-702.

42. *Gasification reactivities of cokes derived from Athabasca bitumen*. **Furimsky.** 11, 1985, Fuel processing technology, pp. 167-182.

43. **Sigma-Aldrich.** [Online] http://www.sigmaaldrich.com/chemistry/stockroom-reagents/learning-center/technical-library/particle-size-conversion.html.

44. Higman, Van der Burgt. Gasification. 2007.

45. **Spirax-Sarco.** [Online] http://www2.spiraxsarco.com/uk/resources/steam-tables/wet-steam.asp.

46. Using Hydrogen as Gas Turbine Fuel: Premixed Versus Diffusive Flame Combustors. Gazzani, Chiesa, Martelli, Sigali, Brunetti. May 2014, Journal of Engineering for Gas Turbines and Power, Vol. 136.

47. *Hydrogen fueled dry low nox gas turbine combustor conceptual design.* **Cerutti, Cocchi, Modi.** Dusseldorf : s.n., 16-20 June 2014. ASME turbo expo 2014.

48. **Cheng, Robert K.** Low Swirl Combustion. [book auth.] U.S Department of energy. *Gas Turbine handbook.* 2006, pp. 241-254.