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**COMPARATIVE ANALYSIS OF ICL AS
AN ALTERNATIVE TO CRUDE OIL**

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Integrative Design of Energy & Mineral Engineering Systems

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Problem Statement

When the US can no longer rely on our current sources of crude oil, how will a domestic indirect coal to syncrude plant compare to other US crude oil alternatives?

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PART 1: INTRODUCTION

The critical role of energy in economic prosperity and environmental quality makes it one of the most important challenges of the 21st century, for the US as well as for the world. In this context the US transportation sector plays an important role as it relies on petroleum derived fuels and it also accounts for about 1/3 of the total green house gas emissions related to the consumption of fossil fuels [1].

Heavy reliance on imported petroleum makes the US economy vulnerable to raising oil prices; therefore energy security has gained increasing attention. The U.S. consumes about 20 Mbbbl of oil every day, of which 60% is imported (12 Mbbbl/day). The share of imported oil has been increasing; in 1990 it was 40% of the total consumption [2]. The transportation sector heavily relies on petroleum derived fuels with as much as 14 Mbbbl of oil consumed every day, 9 Mbbbl of which serve light duty vehicles [2]. In 2008 the price of crude oil “sky-rocketed” to 147\$/bbl, by the end of the year it plunged to 30\$/bbl and since then it has been increasing to today’s value of about 80\$/bbl. The increasing world demand for energy, especially from developing nations, poses concern about the limitations of the resources which is likely to cause an overall increase in energy prices in the long term.

Addressing the issue of security, sustainability and economics of the transportation sector is a difficult task. One single technology might not be able to solve this energy challenge and the possible alternatives to crude oil based transportation are diverse and complex. Alternatives to oil derived fuel are gaining increased interest in the US as well as in the international community. While it is unlikely that one single technology will be able to displace or replace petroleum and solve the issues related to climate change it is important to carefully evaluate all the options for the strongest focus to be placed on the most promising technologies. In this report attention is directed to liquid fuels derived from coal through gasification followed by Fischer-Tropsch synthesis: indirect coal to liquids (ICL). This option is of particular interest because it relies on coal which is the most abundant fossil fuel in the US relative to the rest of the world. According to the EIA, the estimated coal reserves of the US account for 28.3% of the world. Nevertheless, coal is the most carbon intensive fuel and therefore one highly accountable for CO₂ emissions; therefore, the evaluation of carbon capture and sequestration will be taken into consideration in this study. Another aspect of ICL is that it can be easily integrated with biomass as a biomass and coal to liquids (BCTL) process. Biomass is also an important indigenous resource which could have a significant role in tomorrow’s production of fuels and chemicals. Furthermore, biomass as a renewable resource would also have the effect of partly offsetting some of the emissions relative to coal. However, if land is cleared for the production of fuel crops, GHG emissions due to land use change potentially negate the possible benefit. According to the America’s Energy Future Study by 2020 the amount of sustainably available biomass could reach 550 million dry tons per year [2]. Possible pathways are schematically summarized in the figure below.

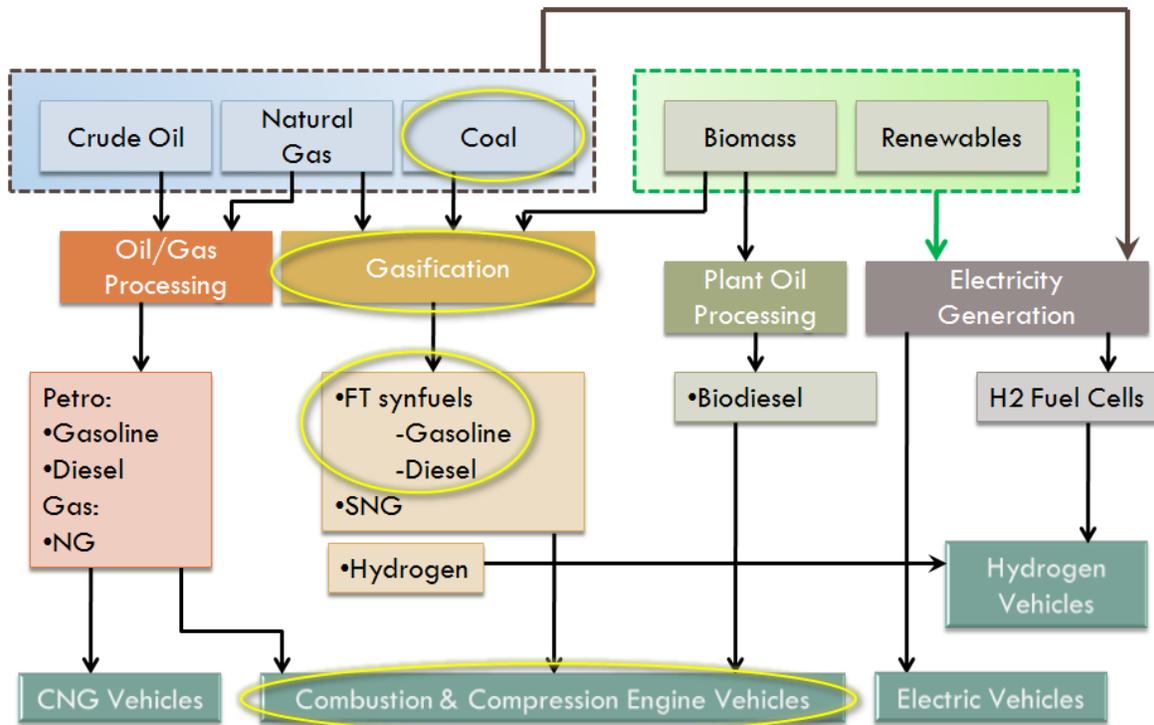


Figure 1 Energy Pathways for Transportation Sector

The objective of this study is to determine the technical and economic feasibility of the implementation of alternative transportation fuels compatible with the current United States infrastructure, and those involving minor alterations, particularly on the demand side. The basis for the comparison will be energy, economics and environmental relative to the modification of the infrastructure, the environmental aspects and the potential for each technology. Special emphasis was placed on indirect coal liquefaction (ICL). With regard to ICL technology, a model plant has been simulated; the location selected is Roxana, IL. The project at hand would use coal from Saline county mines in IL to produce Fischer-Tropsch liquids that will be fed to an in-town refinery for processing into transportation fuels. This study will consider energy, exergy, environmental and economic analysis.

1.1. Status of Indirect Coal Liquefaction (ICL) in the US

Currently, there are no coal-to-liquid fuels commercial plants in the US, but a considerable amount of experience has been gained in coal gasification from the ICL industry established in South Africa by SASOL and from the production of town gas in China, along with other smaller projects worldwide. In the US, the Great Plains gasification plant at Beulah, ND has been in operation since 1984 with fourteen Lurgi gasifiers using North Dakota lignite to produce synthetic natural gas (SNG)[3]. This plant manufactures SNG and other chemical products such as ammonium sulfate and anhydrous ammonia (fertilizers). The process mainly consists in gasification and methanation, producing 153 million cubic feet of methane per day

The only ICL facility currently in operation in the US is the Product Demonstration Unit (PDU) by Rentech Inc[4]. located in Commerce City, Colorado. This demonstration facility produces over 400 gallons per day of synthetic jet fuel, ultra-low sulfur diesel, and specialty waxes and chemicals and is scalable for greater output. The PDU produces synthetic fuels for testing and certification purposes only. A list of some of the proposed CTL projects is shown Table 1 in Appendix A. Most of these projects are under feasibility study, a few others have reached design and construction stages.

A project that appeared close to fruition and initially had extensive DOE support was that of a co-generation plant in Gilberton, PA by Waste Management & Processors (WMP). The proposal was supposed to use around 4700 t/d of anthracite coal waste to produce over 5000 bbl/dof transportation fuels together with 40 MWe of power[5]. The principal products were meant to be an ultra-clean diesel and naphtha which could be upgraded to clean burning reformulated gasoline. For a while, this project faced some environmental opposition and eventually the large capital cost and lack of government support caused the project to be stalled indefinitely in 2008.

1.2. Background

Indirect Coal Liquefaction

The particular focus of this study will be on Indirect Coal Liquefaction (ICL) technology which will be explained in more detail ahead. The term indirect simply refers to first gasifying a feedstock before converting it into liquids via the Fisher Tropsch process. A wide array of ICL technologies exists in order to reach a final product; feedstock preparation equipment, the gasifier, air separation units, syngas cleanup, and the Fischer Tropsch reactor are a few of the major components of any gasification facility.

The obvious advantage of producing synthetic gasoline or diesel (vs. methanol, DME, or other fuels) is that they are compatible with the current infrastructure. Coal to liquid technologies can lead to large life-cycle CO₂ emissions vs. petroleum derived fuels because the H/C ratio of the feedstock must be increased from approximately 0.8 to a desired ratio closer to 2.0. This is done by taking advantage of the water gas shift reaction (WGS) which increases the hydrogen concentration of the synthesis gas from the gasifier, but at the expense of CO₂ production, (CO + H₂O → H₂ + CO₂). A benefit of ICL regarding CO₂ capture is that a stream of relatively pure CO₂ is emitted, owing to the term, “carbon capture ready”. Carbon capture and sequestration is successfully being demonstrated at the North Dakota SNG Gasification facility, where up to two thirds of the daily CO₂ emitted is actually sold for profit at \$7 per ton (at 2200 psi) for use in enhanced oil recovery (Basin Electric, 2008); and as a result is geologically sequestered.

1.3. Overview of proposed ICL Plant

A general process diagram of the proposed ICL is shown in Figure 2. Initially, coal is prepared by milling, grinding and drying operations and then fed to the gasifier where it reacts with steam and an oxidant agent, in this case, pure oxygen, to generate a mixture of gases (mainly CO, H₂ and, CO₂). The gas stream goes through a cooling and cleaning process to remove particulates, sulfur, carbon dioxide and other contaminants by filtration and physical absorption operations, resulting in gaseous mixture of H₂ and CO known as syngas. The syngas is sent through a Fischer Tropsch (FT) synthesis reactor containing an iron catalyst where the synthesis reactor and water-gas shift reaction (WGS) take place simultaneously to produce FT liquids.

The mixture of hydrocarbons from the FT process is referred as 'syncrude'. In the proposed ICL plant design no refinery units will be included since the existing refinery infrastructure in the US will be utilized, thus lowering the capital investment of the ICL plant and allowing an easier transition from current petroleum-based technology into this particular coal-based technology.

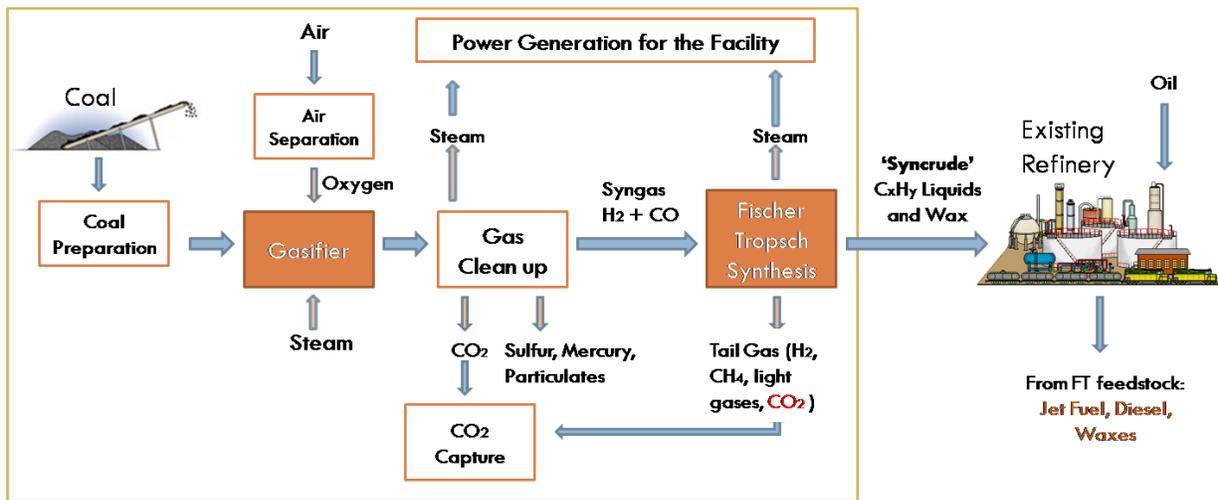


Figure 2 Basic diagram of indirect coal liquefaction (ICL)

The syncrude product would be sent to an existing refinery where it would be hydrocracked and distilled in order to produce middle distillates. A fraction (35%) of the syncrude will consist of naphtha that needs further processing (reforming, catalytic cracking, etc) in order to be able to fit into the gasoline pool. Given that the FT process chosen (low-temperature FT) will generate middle distillates for the most part, diesel is regarded as the main product (after refining) in this analysis.

Based upon the decision to not incorporate refinery equipment in the ICL plant, the US refinery capacity data from late 2009 was carefully reviewed; Figure 3 shows some data from the Energy Information Agency regarding various refining districts (specific state data can be found in the website). It was found that in average most refinery districts work between 80-90% of the total operable refining capacity [6], thus there appears to be enough unutilized capacity for ICL

projects to slowly become integrated into the current oil industry, eventually decreasing the dependency on foreign oil.

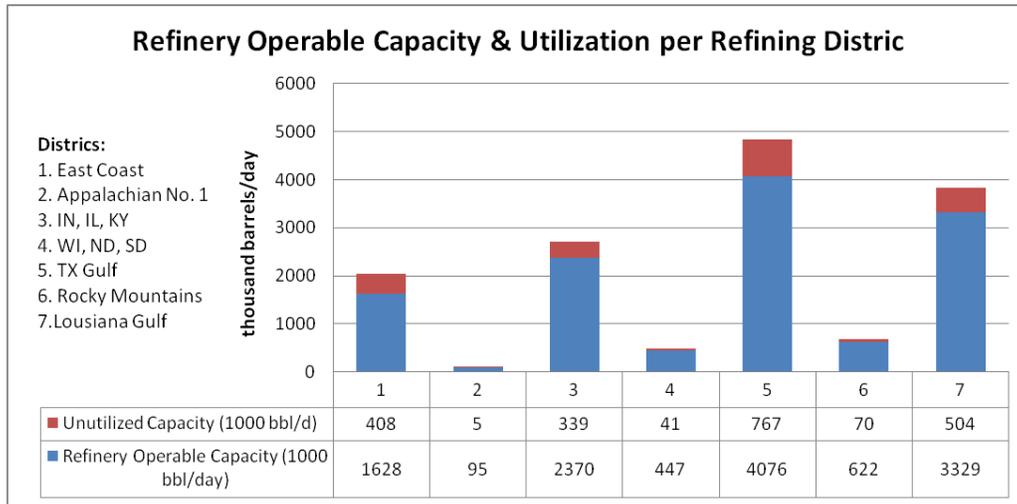


Figure 3 Refinery Capacity Data for various Refining Districts in the US (EIA, 2009)[6]

1.4. Location Selection Process

A geographical/economical/technical analysis was carried out to select a location for a model ICL plant. The site chosen is one of the many places in the US where this technology could be established. A map showing the places that have been previously considered for CTL projects is shown in figure 4.

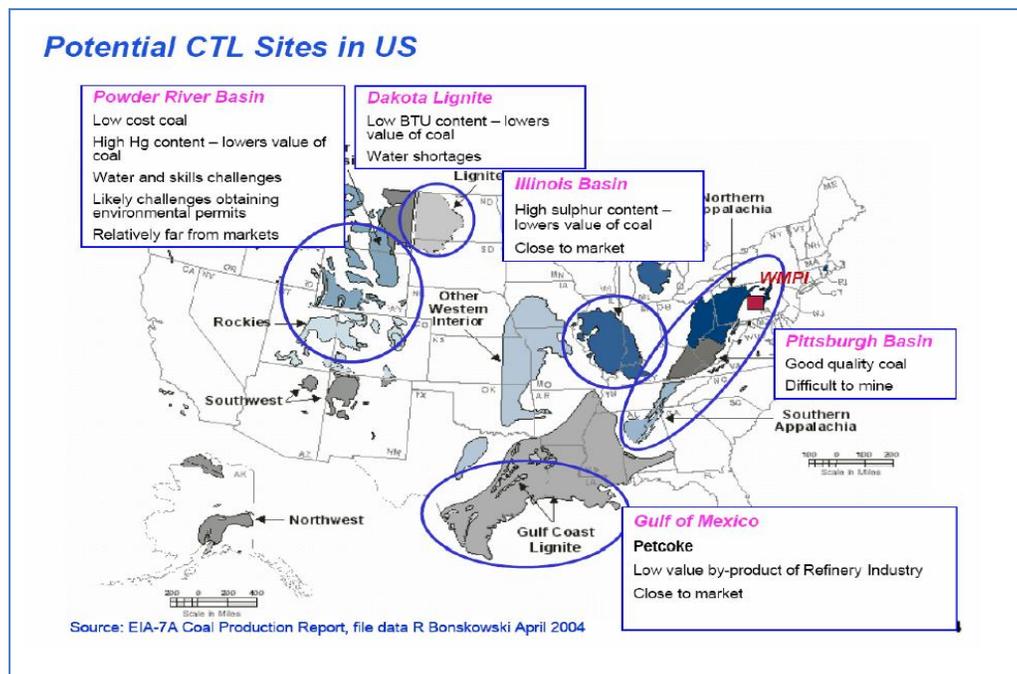


Figure 4 Potential Sites for CTL in the US [7]

Some of the factors considered towards the location selection are listed below:

- ✓ Coal specifications such as coal rank, sulfur content, ash content, heating value and average spot price: the characteristics of the coal define the type of gasification technology that should be used, as well as the performance of the ICL process.

For instance, high sulfur coals are generally considered low-value and less desirable power plant feedstock due to the extra costs associated with the removal of sulfur compounds from the flue gas. ICL *requires* acid gas clean up processes such as Selexol, Rectisol etc, which remove 99% of the sulfur contaminants that would otherwise poison the FT catalysts.

- ✓ Water availability: gasification processes make use of a lot of steam and cooling water. Thus water is an important resource to have in sufficiency near the plant location.
- ✓ Refining capacity: since it is planned to make use of the existing refinery infrastructure in the US, it is essential that the ICL plant is located near a refinery with enough capacity to absorb both the current load of petroleum crude and the 'syncrude' generated by the ICL plant.
- ✓ Mine proximity: accessibility to a coal source that holds the desired coal feedstock is essential to diminish transportation costs.
- ✓ Feedstock transportation means: an already established infrastructure to transport the coal from the mine to the refinery is the key to make the transportation cost-effective. Existing railroad systems to plant location (city) have been considered.

A table showing the locations studied is presented below:

Table 1: Sites considered for construction of proposed ICL plant (Data: EIA website)

LOCATION SELECTION									
PLANT LOCATION	1	2	3	4	6	7	7	8	9
State	IL	IL	TX	KY	PA	PA	PA	WY	OH
City, County	Robinson, Crawford	Roxana, Madison	Atascosa	Catlettsburg, Boyd	Warren, Warren	Warren, Warren	Marcus Hook, Delaware	Casper, Natrona	Canton, Stark
Parameters									
Water Availability	YES	YES	YES	YES	YES	YES	YES	SO SO	YES
Proximity to Refinery	YES	YES	YES	YES	YES	YES	YES	YES	YES
Refinery Capacity (bbl/day)	204,000	306,000	-	226,000	65,000	65,000	178,000	74,000	78,000
Coal Source Location, County									
Coal Rank	Saline	Saline	Atascosa	Floyd	Somerset	Greene	Greene	Sweetwater	Belmont
Price (\$/s.ton) (1)	40.3	40.3	18.6	53.26	65.99	44.97	44.97	26.48	n/a
Sulfur Content (%) daf	2.7	2.7	1.2	0.97	1.4	1.1	1.1	0.72	4.0
HHV (btu/lb) dmmf	11,910	11,910	10,300	15,200	15,800	15,300	15,300	13,200	12,900
other			60% ash						
Transportation for	feedstock	feedstock		feedstock	feedstock	feedstock	feedstock	feedstock	feedstock
Medium	railroad	railroad	-	railroad	railroad	railroad	railroad	railroad	railroad
Distance (miles)	112	150	-	75	150	200	300	100	
MAIN POSITIVE FACTOR	Well known coal seam	Large water availability	Refinery capacity	most resources available		Low sulfur coal	Low sulfur coal	Cheap low sulfur coal	-
MAIN NEGATIVE FACTOR	-	-	Lignite coal, high ash	Higher coal price	Expensive coal	Lower refinery capacity	Large distance from mine	Short water resources	Low refinery capacity
FINAL STANDING	2	1	9	3	7	6	4	5	8

Most of the states under study are known for their coal production (except for TX which is mainly regarded as an oil state), thus the potential plant sites were narrowed down to nine cases based upon those sites that have in-town refineries and that are within a 200 mile radius of producing coal mines. The evaluation was made by weighing the positive and negative factors of the locations and also considering the information available for the coal source, transportation, etc. After considering all the factors, as shown in the “final standing” in table 1, it was decided that the best possible location would be Roxana, IL since it has a large refinery capacity, plentiful water resources and it is rail-connected to the Saline mine county by a relatively short distance. In addition, it was also considered that IL has an overall refinery capacity of 915,600 bbl/d and an operable utilization rate of 84%[6] which means there is around 146,000 bbl/d of unutilized capacity that could be absorb the ‘syncrude’ derived from the proposed ICL plant.

The Galatia mine in Saline County has been chosen as the primary coal source for the facility. The mine produces 7,009,160 short tons annually; and it has been determined that mine output would be sufficient for the lifetime of the plant[6]. The location is such that coal will be delivered via 112 miles of rail[8] and the FT products will be shipped to a local refinery for further processing. The project at hand has sufficient water supply by means of the Mississippi River. Obviously, some water treatment will be necessary prior to using the river water for steam raising and as cooling water in order to avoid solid build-up and contamination of the plant water lines.

1.5. Technical Considerations for an ICL plant (technology overview)

1.5.1. Gasification Technology

There are several basic gasifier designs which have different characteristics; wet or dry feed, air or oxygen blown, reactor flow direction and the gas cooling process. Modern commercial scale gasifiers are capable of processing about 3000 tons of feedstock per day and any given facility can have multiple gasifiers. High temperature, entrained flow design gasifiers produce a glass-like by-product called slag; it is non-hazardous and can be sold for railroad construction, roofing, and other materials. Gasifier designs for lower temperatures produce ash that is a leachable waste product.

When choosing a type of gasifier, the main concern is matching the technology to the feedstock while maximizing the cold gas efficiency (CGE). After choosing the technology and feedstock to be used, the syngas composition (H_2/CO ratio) can be partially controlled by altering the temperature, pressure, H_2O and oxygen ratios, and throughput of the gasifier; the specific details of such will be discussed later.

1.5.2. Entrained Flow Gasifiers

The majority of successful coal gasification processes after 1950 have been achieved using pressurized (20-70 bar), entrained flow, slagging gasifiers operating at temperatures of at least $1400\text{ }^{\circ}\text{C}$ [9]. With respect to the project at hand, entrained flow gasification has also been the preferred gasifier for hard coals. Some of the most advanced gasifiers currently available are the Shell Gasifier, PRENFLO, and the E-Gasifier. High temperature processes of these designs ensure the destruction of tars and oils otherwise present in the syngas, ensuring the highest quality syngas (intended for production of liquid fuels) of any gasifier because of the low methane content.

The primary advantage of using an entrained flow gasifier, (as opposed to fixed or fluid bed gasifiers), is the ability to handle almost any feedstock and produce a clean, tar-free syngas. Additionally, because of high operation temperatures, inert slag can easily be collected. This is considered a by-product rather than a waste product due to marketability of slag. Benefits of entrained flow designs are achieved at the price of high oxygen consumption, thus, the addition of an air separation unit is required. It should be noted that, while, the lowest quality feedstock, (brown coal and lignite), can be gasified in this design, they are most often uneconomical due to excessive moisture and ash content. While moisture content is not a restraint of slurry fed reactors (such as the E-Gasifier); the project at hand has focused on utilization of a dry-fed PRENFLO reactor. The reason for ash limitation is because high temperature slagging gasifiers waste energy melting slag. The ash content of the coal chosen in this study (Illinois #6 coal) is roughly 11% on a dry basis, well within the acceptable limits. [9]

Gasifier Selection

The PRENFLO gasifier has been selected for this project for reasons outlined below. First, it should be noted that methane content of the synthesis gas from the gasifier is undesirable when the final product is to be liquid fuel (as opposed to SNG or IGCC). The increased cold gas efficiency of two-stage and slurry fed gasifiers may be appealing; however, these processes lead to added methane content of the synthesis gas.

The project will favor a single stage, dry feed, entrained flow gasifier for reasons mentioned above; namely the high CO/H₂ composition and low methane content. Particularly, the PRENFLO gasifier with direct quench is favored over the Shell Coal Gasification Process due to decreased capital investment.

1.5.3. Air separation technology

The proposed process requires the gasifier to be fed with a supply of highly pure oxygen (95%-99%). Nitrogen is especially undesirable when the syngas produced is intended for FT synthesis as it would increase the volume of gas to be processed and transmitted and therefore the associated costs. Apart from the decreased size of the gasifier and downstream equipment there are other advantages associated to an oxygen-blown gasifier:

- Smaller volume of gas produced reduces the sensible heat loss from the gasifier;
- The gasifier can be operated economically at higher pressures;
- Heat-exchangers for the recovery of the sensible heat from the syngas are smaller.

For the production of FT fuels the oxygen blown gasifier is currently the chosen method to avoid the presence of large quantities of nitrogen, i.e. the nitrogen barrier[10]. Oxygen makes up 20.3% of the atmosphere (by volume) and can be physically separated from air through an Air Separation Unit (ASU). The technologies available for the separation of oxygen will be briefly reviewed in the following paragraphs. However in order for the design of the indirect CTL plant to be as realistic as possible the choice of the ASU was dictated by the current available and proven technology for large scale operations: cryogenic air separation.

Cryogenic Distillation

Currently the only commercially proven technology for air separation for large scale systems (hundreds of tons per day) is cryogenic distillation. The ASU constitutes a considerable share of the capital cost, as a reference for an IGCC plant cost estimates place the cryogenic ASU and relative compressor between 10-15% of the total plant cost [9].

Cryogenic distillation consists of four main steps:

- Compressing air
- Air impurities removal (including water, carbon dioxide and hydrocarbons)
- Cooling/liquefying

- Distillation (into oxygen and nitrogen)
The products are then heated and vaporized.

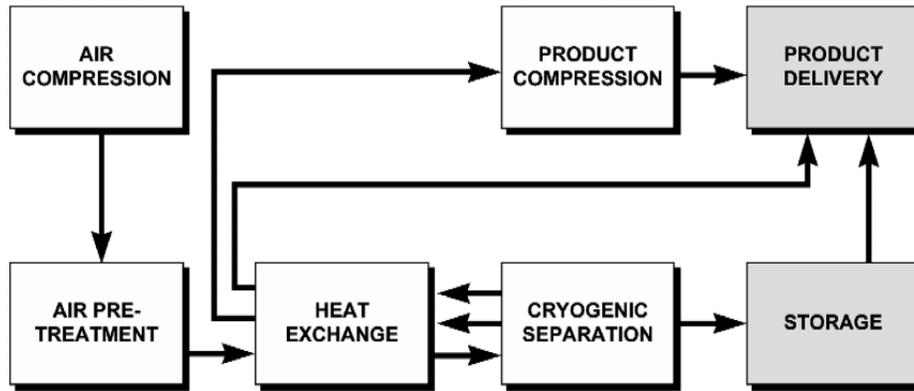


Figure 5 Unit operation for cryogenic air separation [11]

The air pretreatment unit removes water, carbon dioxide (that otherwise would freeze and deposit on the surface of the distillation column) and also hydrocarbons (which is important from a safety point of view). Dangerous contaminants that may be found in atmospheric air include acetylene (the most dangerous), ethane, ethylene, propane, propylene and other hydrocarbons in general, but also oxides of nitrogen and even acetone [12]. Molecular sieves are the typical adsorbents used for pre-treatment. Another option that can be cost effective for smaller production rates are reverse heat exchangers. In this case water and CO₂ are first frozen and then evaporated from the surface of a brazed aluminum reversing heat exchanger [13].

Cryogenics is a general term used to refer to processes that occur at very low temperature, generally below -150°C. Air liquefaction belongs to this category as boiling (liquefaction) of air at 101 kPa occurs at a temperature of -196°C. The cooling and liquefaction of air is obtained through a refrigeration cycle which in general is a process that absorbs heats from the “source” at lower temperature and releases it to the “sink” at higher temperature. This process can be achieved through different methods such as a throttle valve through the Joule-Thompson effect (isoenthalpic process), the expansion in an engine doing external work (ideally isentropic process) and the vaporization of a liquid (isobaric process). Industrial processes use a combination of two or all three methods [10].

The separation of oxygen and nitrogen is obtained through a rectification process. Rectification is based on the principle that when the vapor pressure of two components in a liquid mixture is different (i.e. $p_{N_2} > p_{O_2}$) the component with greater vapor pressure transforms into its vapor to a greater extent. Therefore the concentrations of the two components are different in the liquid and vapor phases. The functioning of the separation column of an ASU can be explained describing the double column process, where a low pressure column is on top of a high

pressure column as represented in Figure 6 Linde's double column process [15]Figure 6. The two section operate at different pressure to achieve heat integration between the two columns to allow energy savings [14]. The pure nitrogen produced at the top of the high pressure column is liquefied in a condenser and fed to the low pressure column serving as a reflux. Oxygen is withdrawn at the bottom of the low pressure column while more volatile nitrogen leaves as a gas from the top.

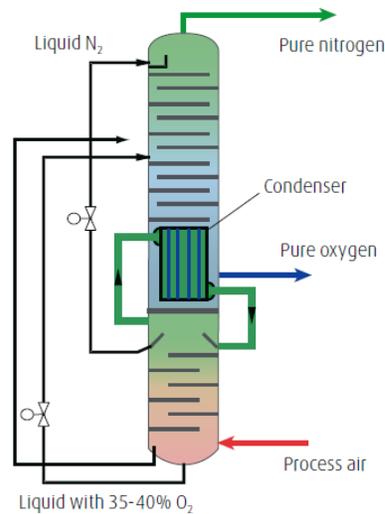


Figure 6 Linde's double column process [15]

1.5.4. Syngas Cleanup

This section will briefly discuss the processes that the syngas will undergo in between the entrained flow gasifier and the FT reactor. In an entrained flow gasifier, the sulfur in the coal is converted to H_2S or carbonyl sulfide (COS). Therefore the main concerns in this system are the removals of hydrogen sulfide and carbonyl sulfide, particulates, carbon dioxide, and hydrogen chloride. For most syngas contaminants the critical aspect of filtering out these undesirables is the compound's (or element's) volatility, hence system temperatures are of large concern. Because of catalyst poisoning concerns, the concentration limits of 1 ppm for particulates and 10 ppb for sulfur compounds must be met before the gas enters the FT reactor [16].

PRENFLO entrained flow gasification occurs at high temperatures ranging over $1500^{\circ}C$ which liquefies almost all the ash. The product gases exit at the top while the slag leaves through the bottom of the reactor where it is quenched in a water bath. The hot syngas is cooled in an internal quench with cold gas and the system is designed in such a way that the cold gas doesn't come in contact with the molten ash. This process brings down the temperature of the syngas to $900^{\circ}C$; however the syngas' temperature is still too high for downstream cleaning processes (particulate and acid gas removal), thus the temperature must be lowered to $400^{\circ}C$ through a cooling-water heat exchanger. Steam generated in this process is used for process

needs in the plant. However, the syngas should not yet be cooled to lower than 280°C in this step because the chlorine compounds in coal form ammonia chloride which in solid form will corrode the cooling equipment[9]. When the syngas temperature reaches around 400 °C it is ready to be cleaned of particulates. A candle filter, where the particulates are captured in a fine grain ceramic layer is used because of its efficiency in removing non volatile elements such as lead and nickel [17]

The two most commonly used acid gas removal systems are the Selexol process and the Rectisol process. Our group has studied both of these and we have found that the Selexol process is best suited for the entrained flow gasification indirect coal liquefaction plant. The main advantages are that it can run at higher temperatures, can cost less, and can efficiently separate CO₂ gas for carbon capture readiness [18, 19], [20]. The first necessary step in acid gas clean-up is to convert the COS into H₂S and CO₂ by COS hydrolysis. The H₂S and CO₂ containing gas stream is sent through an absorber where the Selexol solvent is sent counter current to the syngas stream. The H₂S and CO₂ get absorbed in the Selexol solvent and the clean syngas is sent to the FT reactor. The rich solvent is sent through a stripper where the solvent is regenerated by steam stripping and recycled to the absorber. The H₂S is sent to a Claus plant where the H₂S is oxidized to form elemental sulfur and H₂O.

The Clean Air Mercury Rule is yet to be passed; however, the state of Illinois has its own regulations for mercury limits; hence a mercury reduction technology is included. After looking through different options for mercury reduction Activated Carbon (AC) technology was chosen. A common and well studied AC technology which uses sulfur activated carbon pellets to transform elemental Hg into stable HgS is a very viable option [21, 22]. This process is able to remove 90% of the syngas's elemental mercury, and it has been found that highest removals are obtained at temperatures around 40°C with pressures of 25 bars [23]. Newer activated carbon sorbents loaded with iron compounds have been studied [24] with desired temperatures in the 200-400°C range and lower pressures. This technology benefits from being implemented before other syngas cleaning technologies because other contaminants such as hydrogen chloride and hydrogen sulfide can be beneficial in aiding the mercury reduction.

1.5.5. Fischer Tropsch Synthesis

Fischer Tropsch (FT) synthesis is used for the conversion of syngas to liquid hydrocarbon fuel via surface polymerization reactions over a catalyst. It has been proposed that the reactants CO and H₂ adsorb and dissociate on the catalyst surface to form methylene (CH₂) monomer and water. Hydrocarbons are formed by insertion of CH₂ followed by dehydrogenation or hydrogenation to form olefins and paraffins respectively[25].

Fischer Tropsch Reactions

The reactions that lead to the formation of synthetic liquid fluids in a FT reactor are given below. The H₂/CO ratio as determined from the reaction is between 2 and 3.

Main reactions	
1. Paraffins	$(2n + 1)H_2 + nCO \rightarrow C_nH_{2n+2} + nH_2O$
2. Olefins	$2nH_2 + nCO \rightarrow C_nH_{2n} + nH_2O$
3. Water gas shift reaction	$CO + H_2O \rightleftharpoons CO_2 + H_2$
Side reactions	
4. Alcohols	$2nH_2 + nCO \rightarrow C_nH_{2n+2}O + (n - 1)H_2O$
5. Boudouard reaction	$2CO \rightarrow C + CO_2$

Figure 7 Fischer Tropsch Synthesis Reactions [9].

1.5.5.1. Fischer Tropsch Reactors

The reactor used for FT synthesis is selected based on the temperature of the process as well as the fluidization regime of the catalyst [26]. Large amounts of heat are generated with the FT reactions and insufficient heat removal will result in localized overheating which causes high carbon deposition on the catalysts and subsequent deactivation of the catalyst. The reactor design of FT synthesis is therefore focused on heat removal and temperature control [27], [28].

The temperature and pressure at which the FT reactions occur determine the final product distribution. Higher temperatures favor the formation of smaller chains because of the cracking and less chance of chain growth over the catalyst. Lower temperatures favor the formation of higher molecular weight products. If gasoline and naphtha products are required the reactor needs to be operated at higher temperatures and for the production of middle distillates the FT reactions are performed at relatively low temperatures (220-250 °C).

The best reactors for high temperature FT which is used for the production of gasoline are entrained fluidized bed with riser coolers, such as Sasol's Synthol reactor, and the fixed fluidized-bed with internal cooling coils used at Carthage-Hydrocol plant at Brownsville, Texas [29]. When operating FT at lower temperatures to produce middle distillates as proposed in this project, the above mentioned reactors are not satisfactory because high molecular weight products have fluidization problems. The most feasible options for distillate production are fixed bed tubular reactors and slurry bubble columns.

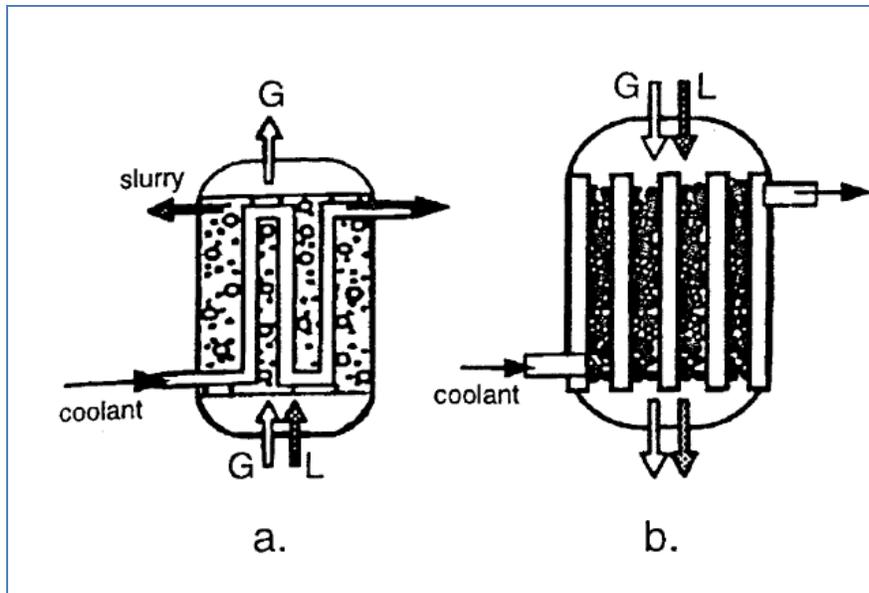


Figure 8 Possible reactors for LTFT: (a) Slurry column, (b) Multitubular Fixed bed [G: Gas, L: Liquid] [27]

Sasol has used a fixed bed tubular design, called ARGE at a high capacity for many years now. Shell also uses a multi-tubular fixed bed reactor for production of middle distillates in Malaysia [26]. The reactor has between 10 and 100 000 tubes which are filled with catalyst and immersed in water for temperature control. The syngas flows through the tubes from the top of the reactor and the product exits at the bottom consisting of up to 50% wax. The reactor is operated at 20-30 bar at an operating temperature of 220-260 °C. Additional temperature control is obtained by using high gas velocities and gas recycling.

The alternative to the fixed bed is a slurry bubble column which has also been used by Sasol [30] as well as by Exxon and Rentech Inc. The slurry phase reactor is a three phase reactor consisting of solid catalyst suspended in a liquid, often FT wax products, with the syngas bubbling through [26]. The slurry phase is well mixed resulting in isothermal conditions which gives much easier temperature control. This, together with better catalyst dispersion, results in a higher single pass conversion compared to the ARGE reactor. Even though the construction cost of slurry phase reactors are expected to be lower without the expensive tubes, the up scaling is not as straightforward and safe as with the fixed bed tubular design. Another disadvantage of the slurry design is its lack of capability to handle poisons in the syngas [29]. All the catalyst in the reactor will be affected while only the catalyst near the gas inlet will be poisoned in a fixed bed design. The slurry phase reactor also requires continuous separation between the catalysts and liquid which is a major drawback [31]. Attrition of the catalyst is another problem with slurry columns but on the other side a slurry bed needs about a third of the catalyst loading of a fixed bed [29]. After careful consideration, the multi-tubular fixed bed reactor was chosen as the most suitable for this project.

1.5.5.2. Fischer Tropsch Catalysts

Group VIII transition metal oxides are generally good CO hydrogenation catalysts. Of these, ruthenium has the highest activity as well as a good selectivity for producing high molecular weight products [32]. It is however also the most expensive of the possible catalysts and therefore not a feasible choice. Nickel has a good activity but the tendency to promote the formation of methane which is undesirable. Iron is the most commonly used catalyst and can use synthesis gas with a low H_2/CO ratio since the excess of CO is converted with water to carbon dioxide and hydrogen in the water gas shift (WGS) reaction. Although this reaction results in formation of unwanted CO_2 , it shifts the H_2/CO ratio of the incoming synthesis gas [26]. This is especially important for synthesis gas derived from coal, which tends to have a ratio of ~ 0.7 compared to the ideal ratio of ~ 2 . Fe catalysts are good water gas shift catalysts and the need for a separate WGS reactor can be eliminated if an iron catalyst is used in the FT reactor. Cobalt-based catalysts are also used in industrial applications but due to its low selectivity for the WGS reaction it is only suitable for a feed such as natural gas which has a high H_2/CO ratio. Cobalt catalysts could still be used but a separate WGS reactor would be needed prior to the FT synthesis reactor which increases the capital cost. The best cobalt catalysts are supported ones, while the best iron catalysts are the precipitated ones [33]. This results in a higher metal area for iron catalysts compared to cobalt catalysts. Therefore even though cobalt has a higher turnover per active catalyst site, the higher density of iron sites per unit surface area results in a higher overall activity. Taking all these issues into account an iron-based catalyst will be used in our design.

PART 2: ICL PLANT SIMULATION AND ANALYSIS

This part of the report includes the methodology, assumptions and results from Aspen simulation of the ICL plant. Also included are the results for biomass gasification and the sensitivity analysis. The Aspen simulation was used to set up the mass and energy balances over the ICL plant which is also included in this section. Methodologies used to perform the exergy and economic analyses as well as the results achieved are also discussed in this section. In addition the environmental analysis of the plant and a discussion on the applicable policies and government support are included in this section.

2.1. Aspen Simulation of ICL

Aspen PlusTM is a software package that was used to simulate the indirect coal liquefaction plant. The simulation results were used to do a mass, energy and exergy analysis over the CTL plant. The results were also used as inputs into the economic model. A sensitivity analysis was performed by changing process variables to analyzing the effect it has on process outputs.

2.1.1. Methodology

Illinois #6 coal and herbaceous biomass (switchgrass) was simulated as nonconventional solids as suggested in Aspen Plus' tutorials [34]. To define a nonconventional solid, the following fields had to be completed with values found in table below: proximate analysis, ultimate analysis, sulfur analysis, and heating value. The Peng-Robinson equation of state was used to determine the thermodynamic properties of the components in the simulation.

Table 2 Gasifier Feedstock Properties

	Illinois #6 coal (dry basis)	Switchgrass (dry basis)
Proximate Analysis		
Fixed Carbon	49.72	15.0
Volatile Matter	39.37	81.4
Ash	10.91	3.6
Ultimate Analysis		
Carbon	63.75	46.96
Hydrogen	4.5	5.72
Oxygen	6.88	40.18
Chlorine	0.29	0.86
Sulfur	2.51	0
HHV (MJ/kg)	30.56	18.65

A diagram of the entire process simulation is shown in Appendix B. The various segments of the plant that were simulated, shown in the figure in the appendix, will be explained individually in the following sections.

2.1.1.1. Gasifier Simulation

Even though Aspen Plus has been used to model gasifiers in the past, gasifier modeling continues to be challenging. Selecting a gasifier model depends on the accuracy and robustness required [35]. Aspen Plus was used to model the entrained flow gasifier by dividing gasification into the main mechanisms occurring in the reactor. The model has essentially three steps: (1) decomposition of coal; (2) conversion of elements to gas-phase components; and (3) equilibration of the gas-phase components. This type of modeling approach has been proven to give results comparable with experimental values [36, 37].

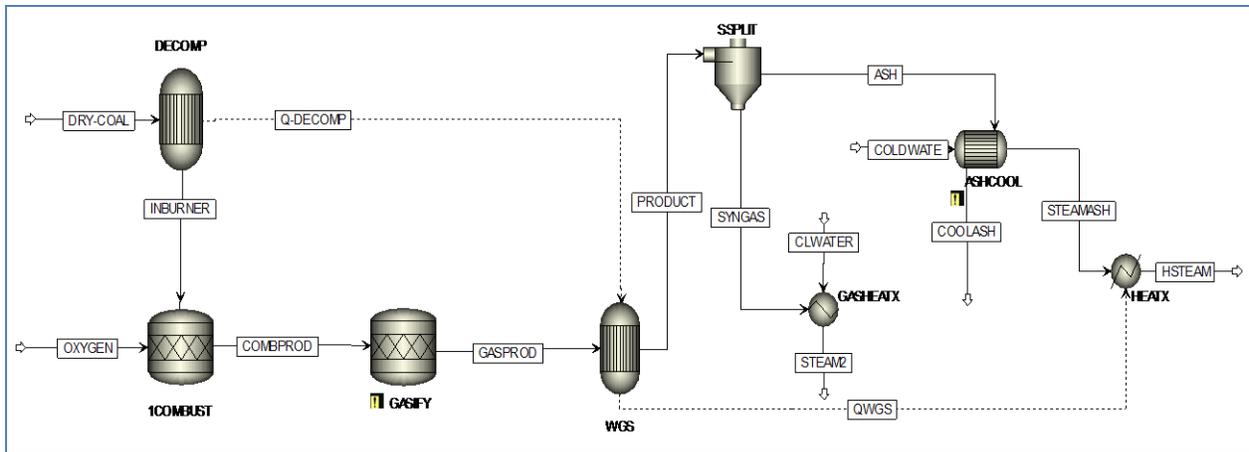


Figure 9 Gasifier simulated in Aspen Plus

A FORTRAN subroutine together with an *RYield* reactor was used for the decomposition of coal into its constituent elements and ash based on the ultimate analysis [34]. The elemental coal constituents are then mixed with the gasifier O_2 in an *RStoich* reactor block (COMBUST in Figure 9), where all the O_2 is converted to CO_2 . The unconverted carbon and the elemental sulfur react with steam in a second *RStoich* to form CO , H_2 and H_2S . The final step of gasification occurs in an *RGibbs* reactor (labeled WGS in Figure) where all the constituents are brought to equilibrium.

Heat generated from the gasifier is extracted using a heat exchanger where water at $25\text{ }^\circ\text{C}$ is fed and low quality steam at 1 bar and $180\text{ }^\circ\text{C}$ is generated. This simulates the cooling system of the gasifier. The ash, as slag, is separated from the gases using *SSplit* block. The gases are then cooled down to $500\text{ }^\circ\text{C}$ using a heat exchanger which generates high quality steam. The slag is also cooled and steam is produced.

2.1.1.2. Gas cleanup

The gas cleanup section includes various steps; a candle filter, COS hydrolysis, Selexol and the Claus process.

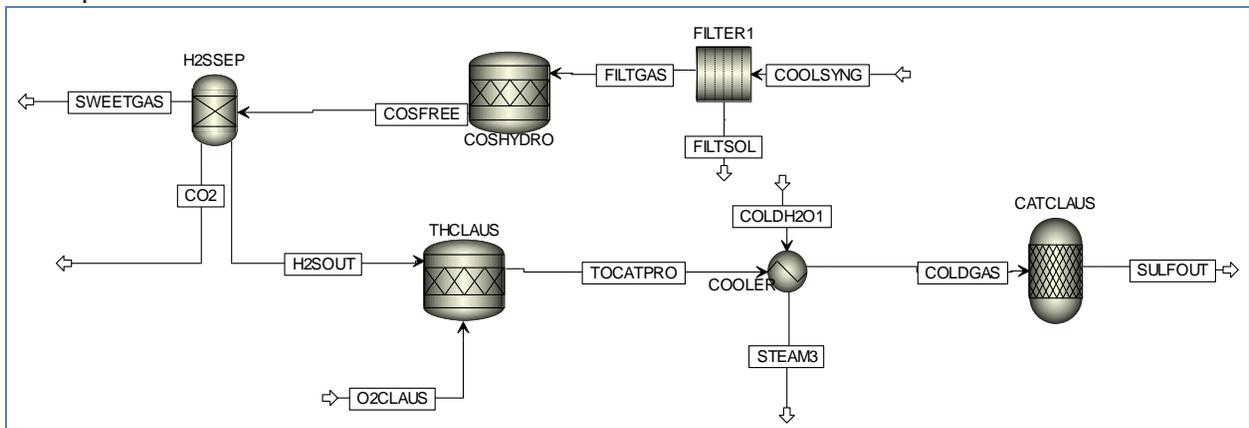


Figure 10 Gas cleanup simulated in Aspen Plus

A filter in Aspen was used to remove any particulate matter present in the gas. The COS hydrolysis step was simulated using an *RStoich* reactor block and the conditions for the process were taken from literature [38]. The Selexol process was proposed as the gas clean up technology for our plant. Since the Selexol process is a proprietary process we were not able to get the data to simulate the process accurately. The Selexol process was simulated as an ideal process using a SEP block where 99.99% H₂S and 95% of CO₂ were removed from the cool syngas. The H₂S was then sent to a Claus plant where elemental sulfur is formed. The Claus plant was also modeled as an ideal process with two *RStoich* reactor blocks operating at 1200⁰C and 250⁰C respectively [39, 40]. The first *RStoich* block was used to simulate the thermal Claus process where a part of the H₂S is converted to SO₂. The second *RStoich* block simulated the catalytic Claus process where the SO₂ and H₂S react to form elemental Sulfur. Even though the material balance around the gas cleanup process was right, the energy balance is not completely accurate since ideal separators and reactors were used.

2.1.1.3. Fischer Tropsch synthesis

The clean syngas was split into two streams; 12% and 88% by mass which were sent to a gas turbine and the FT reactor respectively. A plug flow reactor (*RPfr*) was used to model the multi-tubular fixed bed FT reactor operating at 270⁰C and 2 bar. An iron catalyst with an apparent density of 647 kg/m³ [41] and a loading of 850 kg was used in the reactor. Steam was generated from cooling the reactor and the product. After the product was cooled down a phase separator was used to separate the FT products from the gasses.

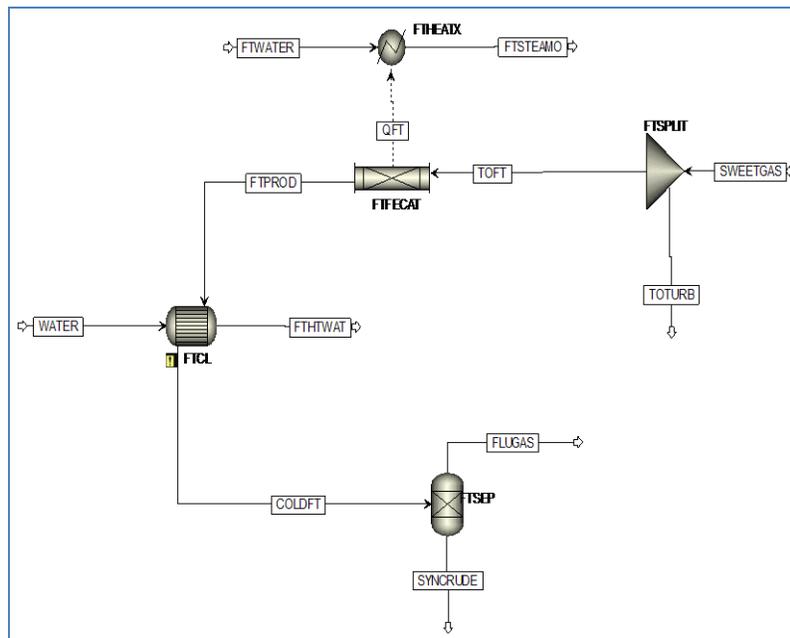


Figure 11 Fischer Tropsch synthesis simulated in Aspen Plus

A kinetic model [41],[42] involving both the FT and the WGS reactions was used to describe the overall performance in the reactor. Reaction rate equations based on Langmuir–Hinshelwood–Hougen–Watson models are given by:

$$R_{\text{FTS}} = \frac{k_{\text{FTS}} P_{\text{CO}} P_{\text{H}_2}}{P_{\text{CO}} + a P_{\text{H}_2\text{O}}}$$

$$R_{\text{WGS}} = \frac{k_{\text{WGS}} \left(P_{\text{CO}} P_{\text{H}_2\text{O}} - \frac{P_{\text{CO}_2} P_{\text{H}_2}}{K_1} \right)}{(P_{\text{CO}} + K_2 P_{\text{H}_2\text{O}})^2}$$

The kinetic parameters and assumptions of the model can be found in the Appendix C. By using product distributions from literature [43] it was determined that n-undecane could be used as the average molecule composition of the LTFT product.

2.1.2. Model Assumptions and Limitations

The gasification reactions were modeled in four separate reactor blocks. The first three reactor blocks are assumed to be adiabatic reactors while the last reactor block of the gasifier, where the products of gasification are brought to equilibrium, is assumed to be isothermal. In an actual gasifier there is a temperature gradient across the gasifier with the region in which the reactions take place being isothermal. The major limitation of this gasifier model is that it does not take into account the flow regimes inside the gasifier. The temperature and pressure at which the gasifier model operates at determines the type of gasifier. Tar formation in the case of biomass gasifier was not considered. Heat losses from the gasifier to the environment were also not considered.

The COS hydrolysis reaction which converts COS to H₂S was modeled in an *RStoich* reactor block. This reactor block doesn't take into account the kinetics of the reaction and hence the heat balance over that block may be inaccurate. The H₂S and CO₂ separation which takes place in the Selexol process was also not modeled because of lack of information about the Selexol solvent. Hence in place of absorbers and strippers we have a *Sep* block which does an ideal separation; therefore, the heat balance for this process is not accurate and the process water consumed here is not considered in the overall plant water usage. The Claus process where the H₂S is converted to elemental sulfur was modeled using two *RStoich* blocks; therefore, the material balance would be accurate but the energy balance might not be representative of the real process. The steam requirements as well as the solvent used for the Selexol process were not considered. This is a major limitation of our model. The entire gas cleanup section was modeled as a series of ideal processes; hence the efficiency of our plant is higher than an actual plant.

The FT synthesis reactor was modeled as a PFR with a 100 % conversion of H₂. A sensitivity analysis on the length of PFR shows that the H₂ is consumed within 0.5 m of the reactor, which might not be the case in a real system. This might be because we have taken the syngas produced only from one gasifier as opposed to 8 gasifiers used in the actual plant to produce the 50,000 bbl/day. Another limitation of our model was that we have not modeled the Anderson-Schulz-Flory distribution. Instead of a product distribution we get a single product; therefore, the efficiency we calculate for our whole plant increases. This affects the exergy analysis as well since the chemical exergy changes if there is range of products instead of just one. No heat losses to the environment were taken into account in the model.

The results from the Aspen simulation are shown in the following table. As it was mentioned before the efficiency resulted slightly higher since some of the processes were treated as ideal processes and the refinery steps for the product were not simulated.

Table 3 Simulation results

Feed	100% Coal
Syngas composition	CO: 59.5% H ₂ : 30.7%
FT product	29.6 t/hr
Efficiency	51.2%

2.1.3. Biomass gasification

For comparison purposes, a biomass-to-liquid (BTL) and a coal-biomass-to-liquid (CBTL) were also simulated in Aspen Plus. Switchgrass was used as biomass feedstock since it is available in the Roxanna, IL area [44]. A circulating fluidized bed (CFB) gasifier was selected for gasifying switchgrass with 10% moisture content and to co-fire a mixture of 25% switchgrass (10% moisture) and 75% coal. Other than changing the operating conditions to 900 °C and 1bar in the gasifier [9], there were no changes in to the ICL simulation .

Table 4 BTL and CBTL simulation results

	BTL	CBTL
Feed	100% Switchgrass	25% Switchgrass 75% Coal
Syngas composition	CO: 41.6% H ₂ : 36.5%	CO: 53.3% H ₂ : 33.1%
FT product (t/hr)	17.8	29.2
Total CO ₂ emissions (kg CO ₂ /GJ product)*	-6.7	86.2
Efficiency	50.8%	51.3%

* Assuming that biomass has a storage capacity 17.2 kg Ceq/GJ HHV [43]

2.1.4. Sensitivity analysis

In order to test the robustness of our simulation a sensitivity analysis was performed by varying the oxygen and steam input into the gasifier. The O₂ flowrate was varied from 17 kg/s to 40 kg/s while the steam flowrate was kept constant at 7.2 kg/s. The steam flowrate was varied from 3 kg/s to 11 kg/s while the O₂ flowrate was kept constant at 23.87 kg/s.

As seen in Figure 12 the CO and H₂ molar flows in the syngas increase as oxygen flowrate decreases. The increase in the molar flow of H₂ at a lower O₂ flowrate can be attributed to the fact that there is unreacted coal which reacts with the steam to generate H₂. The red arrow in the graph represents the minimum O₂ flowrate at which the gasifier needs to be operated for the reactions to occur without additional heat. As the O₂ flow rate increases the amount of CO and H₂ formed decreases and there is an increase in the formation of CO₂ which can be expected. The amount of water exiting the gasifier also increases as the O₂ flowrate is increased because the reaction of coal with O₂ is faster and thermodynamically more favorable than the reaction of steam with coal.

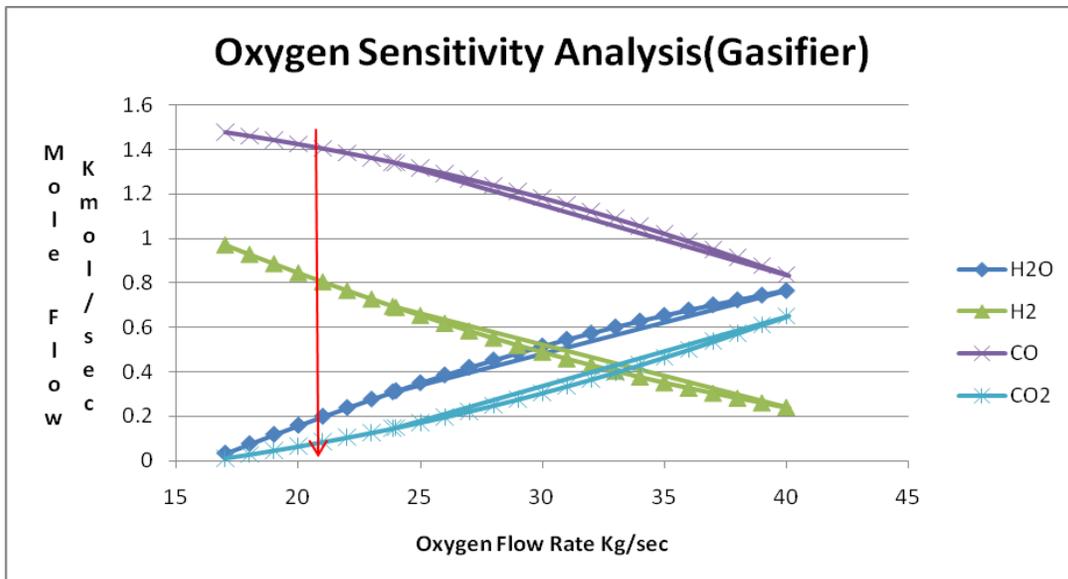


Figure 12 Oxygen Sensitivity Analysis

The sensitivity analysis with steam shows interesting trends. As the steam flow rate is increased the CO flowrate decreased while the H₂, H₂O and CO₂ flowrate increased. This shows that the forward water gas shift reaction ($\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$) is a probable cause for the trend seen in Figure 13.

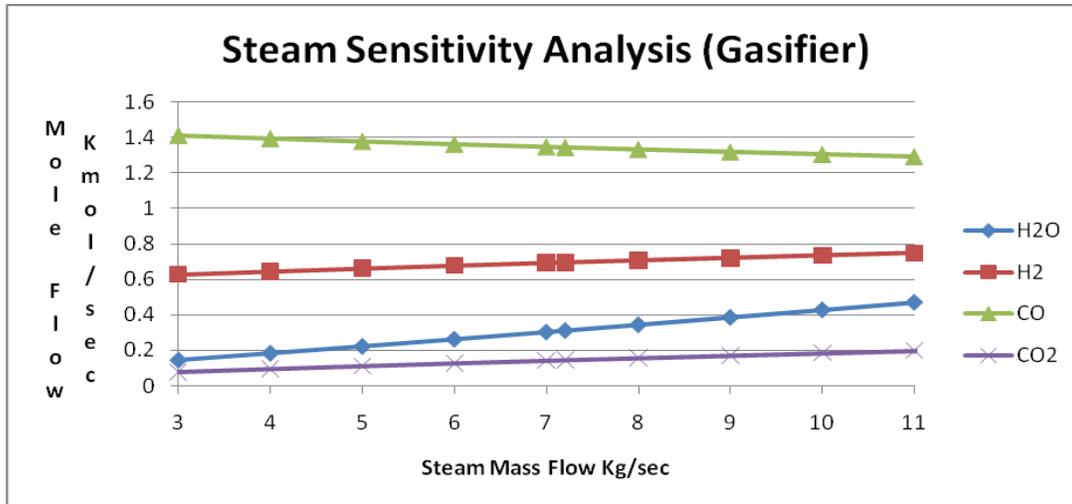


Figure 13 Steam Sensitivity Analysis

When a graph is plotted between the steam input and the H₂O in the exiting syngas and the values are extrapolated to zero steam flowrate, it is seen that there is some H₂O in the exiting gas and the cause might be the reverse water gas shift reaction, which would result in an increase in CO and H₂O flowrates.

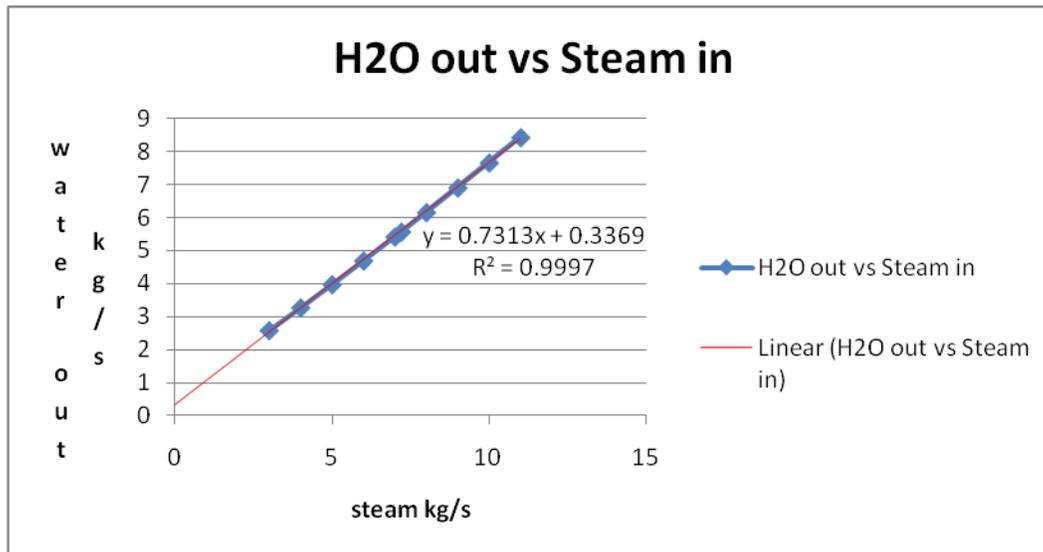


Figure 14 Water out compared to steam in

2.1.5. Suggested improvements for Aspen Plus simulation

Future work should include the modeling of pumping, compression, electricity generation, activated carbon column for mercury removal, milling, grinding and other feedstock preparation steps. To improve the current model the following should be included:

- Obtain data on the Selexol solvent to accurately model the Selexol process as an absorption process.
- Use FORTRAN to write a subroutine that will model the FT product formed by using the Schulz-Flory-Anderson distribution.
- Reaction kinetics for Claus process and COS hydrolysis.
- Heat recovery and integration from exothermic processes.

2.2. Exergy and Energy Analysis of the simulated ICL plant

The approach chosen for the detailed analysis of indirect CTL is that of exergy analysis. Exergy allows the quantification of efficiency losses in terms of losses in the quality of energy, namely the potentially available work. Therefore, exergy analysis detects the causes of thermodynamic imperfection of thermal and chemical processes which are completely transparent to an energy analysis and by doing so it provides information on where the process can be qualitatively and quantitatively improved. The methodology adopted for the study is based on Jan Szargut's monograph "Exergy analysis of thermal, chemical and metallurgical processes" [45] which is considered the standard reference in the field, though it does not represent the only way to compute an exergy analysis.

In the following paragraphs the main concepts underlying exergy analysis will be outlined along with some of the key equations we are using in this first approach. The major assumption at the moment is the ideality of the gases involved.

2.2.1. Overview of Exergy Analysis: "the fight against irreversibilities" (F. Bosnjakovic)

The definition of Exergy according to Szargut is: "*Exergy is the amount of work obtainable when some matter is brought to a state of thermodynamic equilibrium with the common components of the natural surroundings by means of reversible processes, involving interaction only with the above mentioned components of nature.*"

Exergy, unlike energy, is not conserved because of the production of entropy associated with processes that are not reversible. Exergy depends both on the state of the system and its natural surroundings. Consequently, while energy may be calculated on the basis of any reference state, for exergy the reference state is imposed by the environment which may vary. Another important difference between energy and exergy is that the former always increases with temperature while the latter for an isobaric process reaches a minimum at the temperature of the reference environment. For an ideal gas energy does not depend on pressure while exergy always does. This leads to a positive exergy of an ideal vacuum while its energy is zero.

The components of exergy are kinetic, potential, and thermal. Kinetic exergy is equal to the kinetic energy and potential exergy is equal to potential energy. Thermal exergy has two components, physical and chemical.

$$B = B_k + B_p + B_{th} \quad B_{th} = B_{ph} + B_{ch} \quad (1)$$

In the exergy analysis of indirect coal liquefaction, kinetic and potential exergy will not be taken in consideration as the main components of interest for the process are chemical and physical exergy.

Physical exergy is the work obtainable by reversibly taking a substance from its initial T and p, to the conditions of the environment: T_o and p_o. The change in exergy is equivalent to the change in Gibbs free energy. For an ideal gas with a constant heat capacity physical exergy can be expressed by the following relationship:

$$b_{ph} = \Delta g(p, T) = c_p((T - T_o) - T_o \ln \frac{T}{T_o}) + RT_o \ln \frac{p}{p_o} \quad (2)$$

Chemical exergy is the work obtainable by taking a substance at T_o and p_o to the state of thermodynamic equilibrium with the datum level of the components in the environment. But because the earth itself is not in thermodynamic equilibrium, the concentration of chemical species must be defined by a standard. For example, Ahrents [45] studied what the composition of the environment would be like if increasing layers of the earth crust were to achieve thermodynamic equilibrium. The composition that would arise in such a “dead state” would be very different from the actual composition of the environment and therefore it cannot be considered as a reference state. The reference environment for this study is the one defined by Szargut, who introduced the concept of standard chemical exergy at normal temperature and pressure (298K, 101.325 kPa) partitioning the earth in sea water, air and crust and who tabulated the standard exergy for an extensive collection of compounds. For a hypothetical ideal gas the *standard chemical exergy* is:

$$b_{ch}^0 = RT_n \ln \frac{p_n}{p_{on}} \quad (3)$$

Where T_n and p_n denote the conditions of the standard environment. In general, if high accuracy is not required, *chemical exergy* can be approximated with the *standard chemical exergy*.

The formation of a solution is always an irreversible process and therefore denotes an increase in entropy (i.e. a reduction in Gibbs free energy) which must be taken into consideration. The total chemical exergy can be expressed as:

$$B_{ch} = \sum n_i b_{ch} + RT_o \sum n_i \ln (a_i) \quad (4)$$

Where the second term is always negative and a_i represents the activity which for an ideal solution is equal to the mole fraction.

2.2.2. Exergy of Fuels

ICL aims at transferring the exergy contained in coal to liquid fuels, a more practical “exergy carrier.” Calculating the exact chemical exergy of fuels is a challenging task which can become impossible for complex fuels such as coal. This study will rely on the statistical method proposed by Szargut and Styrylska [45] to calculate the exergy of the specific coal and biomass used and that of the fuel produced. This method expresses the dependence of the ratio between the net calorific value of the fuel C_i^0 and the standard chemical exergy as a function of the elemental composition of the fuel through the parameter β . The chemical exergy of a fuel can therefore be expressed as:

$$b_{ch} = (LHV + Lz_w)\beta + (b_{chS} - C_s)z_s + b_{cha}z_a + b_{chw}z_w \quad (5)$$

Where:

LHV is the net calorific value of the fuel

L is the heat of vaporization of water

z_w, z_a, z_s are the moisture, ash and sulfur content of the fuel (mass fraction)

$b_{chS} - C_s$ calculated from the standard values is 9683 kJ/kgS

b_{cha} is the standard chemical exergy of ash which can usually be neglected

b_{chw} is the standard chemical exergy of water

The equations for β proposed by Szargut and used in this study are reported hereunder:
For bituminous coal, lignite, coke and peat:

$$\beta = 1.0437 + 0.1896 \frac{z_{H_2}}{z_C} + 0.0617 \frac{z_{O_2}}{z_C} + 0.0428 \frac{z_{N_2}}{z_C} \quad (6)$$

For biomass:

$$\beta = \frac{1.0412 + 0.2160 \frac{z_{H_2}}{z_C} - 0.2499 \frac{z_{O_2}}{z_C} \left[1 + 0.7884 \left(\frac{z_{H_2}}{z_C} \right) \right] + 0.0450 \frac{z_{N_2}}{z_C}}{1 - 0.3035 \frac{z_{O_2}}{z_C}} \quad (9)$$

For liquid fuels:

$$\beta = 1.0435 + 0.0159 \frac{H}{C} \quad (8)$$

The coal used for all the analysis in this study is Illinois #6 coal. The biomass considered for the sensitivity analysis of the gasifier and overall plant is switchgrass. The proximate, ultimate analysis, calorific values for the fuel inputs are reported Table 2. The exergy values calculated are summarized below.

Table 5 Exergy content of fuels

	b_{chem} [MJ/kg]
Coal, Illinois #6 (dry)	31.580
Biomass, switchgrass (10 % moisture)	17.76
Syncrude, undecane	47.37

2.2.3. Approximate exergy and energy analysis of our model ICL plant

Many publications on biomass, coal and gas to liquid conversion report energy balances and life cycle analyses based on first law efficiencies. Recent studies have addressed the exergy analysis of BTL [46] [47] [48] conversion and gas to liquid (GTL) processes [49] but to the best of our knowledge the only study where the second principle of thermodynamics is applied to coal to liquids conversion appeared in a 1982 publication by Nishida and Ishida titled “Evaluation of coal conversion processes from an energy efficient use viewpoint. (IV) - Energy and exergy analysis of liquefaction process” [50] which unfortunately is available only in Japanese.

The exergy and energy analysis carried out on the ICL plant model are inherently affected by many approximations. As explained before, the physical exergy of the gaseous streams was approximated to that of ideal gases with equation (2). In the case of steam the physical exergy was calculated from the Aspen values of enthalpy and entropy. To further simplify the calculations the reference environment was considered at the standard conditions of 25°C and 101.325 kPa. Other sources of approximation derive from the modeling of our plant. As explained in section 2.1 some of our processes were modeled as “black boxes” for which the energy balances are not representative of real processes. Furthermore, a real plant is optimized using process integration which we took into account just to a limited extent. For example the FT reactor requires cooling and therefore steam is produced which might be used in other sections of the plant. In the proposed model though heat integration wasn’t taken into account and therefore the steam produced is referred as a loss relative to the FT reactor. In reality the steam is used in other processes after its quality is raised in a boiler. This important approximation could not be overcome at this stage and it does affect the partition among processes of the energy and exergy losses of our plant represented in Figure 19 and Figure 20. Nevertheless, the Grassman diagrams (Figure 18 and Figure 17) show that the bulk of the exergy and energy is represented by the fuel streams (coal, syngas and syncrude) while all other streams are much smaller and therefore the main streams are well characterized in this analysis. Even so a thorough exergy analysis should account for all the streams in order to correctly assess where the process could theoretically be improved. This is why we do not claim the results to be applicable to indirect coal liquefaction in general and a more in depth study would be necessary to verify our conclusions. Nevertheless, this analysis allows the evaluation of the differences that arise by applying exergy and energy analysis to this system and to track the energy and exergy changes in the main streams.

2.2.4. Results of Mass, Exergy and Energy Analysis of ICL model plant

In order to carry out the analysis the ICL plant model was divided into four main sections:

- Gasifier
- Ash cooling
- Syngas cooling, filtering and cleaning
- FT synthesis

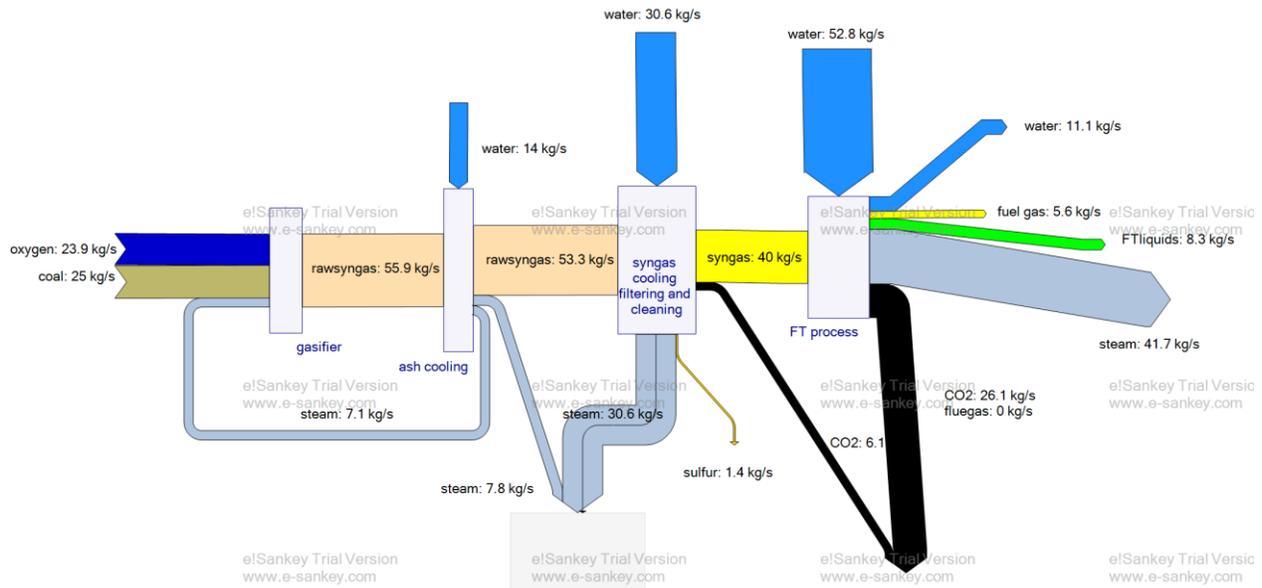


Figure 16 Mass flow diagram of modeled ICL plant

The energy and exergy Grassman diagrams are represented in Figure 17 and Figure 18 respectively. For the energy analysis of the streams the high heating value (HHV) of the fuels was taken into consideration (for coal, syngas and syncrude) as well as their physical enthalpy. The first difference arising from the comparison of energy and exergy streams is that in the latter case streams like oxygen, sulfur and carbon dioxide acquire a greater importance. Their exergetic content, as explained before, takes into account the difference in concentration with the reference environment. Furthermore, in the exergy analysis streams with the same “quality of energy” are being compared while in the energy analysis heat and electricity streams are treated equally. On the other hand exergy and energy values of the main fuel streams (coal, syngas and syncrude) are similar as the chemical energy content of a fuel it is similar to its exergy.

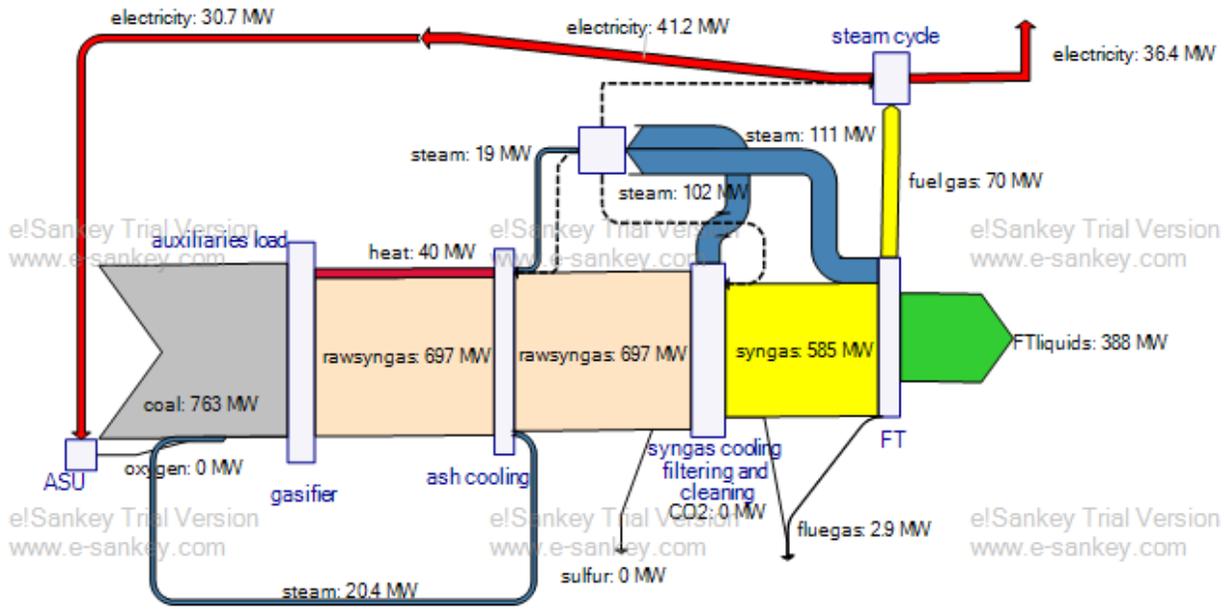


Figure 17 Energy flow diagram of modeled ICL plant

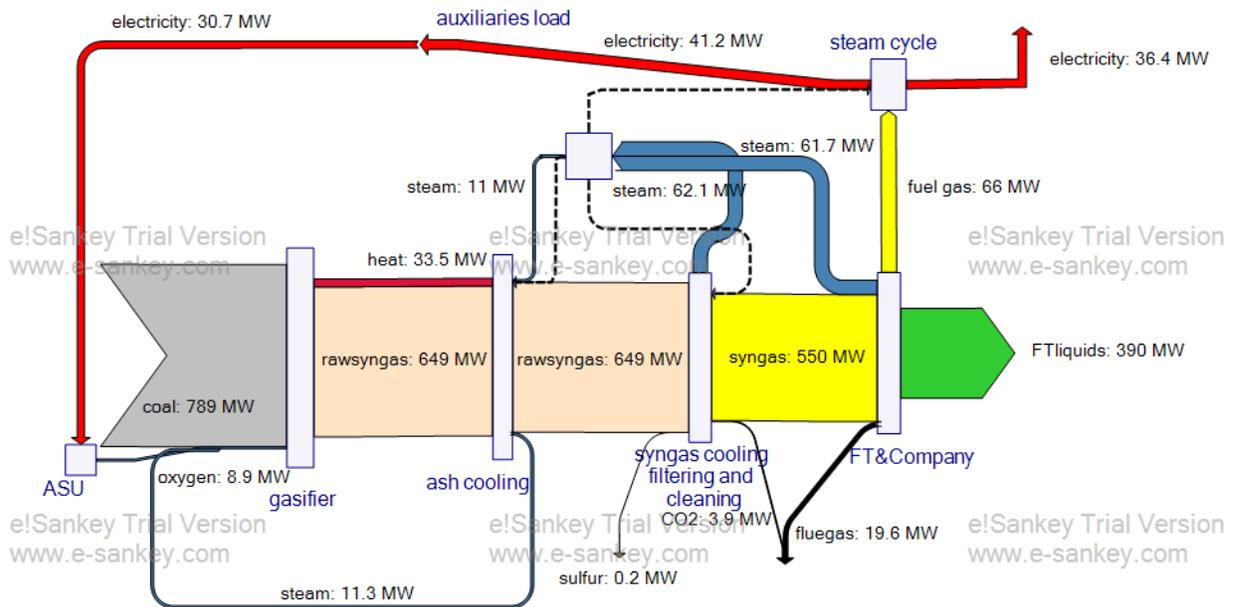


Figure 18 Exergy flow diagram of modeled ICL plant

For the overall analysis of the plant the inputs and outputs of every section were analyzed to determine their contribution to the overall efficiency. The losses are constituted, a part from the non-ideality of certain components (like the heat exchangers), by the reduction in the

chemical energy of the streams, for example with the production of carbon dioxide which has to be removed from the system. The pie charts reported in Figure 19 and Figure 20 represent the overall energy and exergy analysis of the plant, respectively. In these figures the pie chart on the left represents how the energy/exergy input (i.e. the coal) is partitioned between useful outputs (i.e. the FT syncrude and electricity) and losses. The chart on the right represents where the losses occur in the system, which is the difference between inputs and useful output of every process. The *delta* value refers to the difference between the value for losses obtained by subtracting the energy/exergy output to the energy/exergy input and the value for losses obtained by summing the losses relative to every single process. Ideally *delta* should be zero.

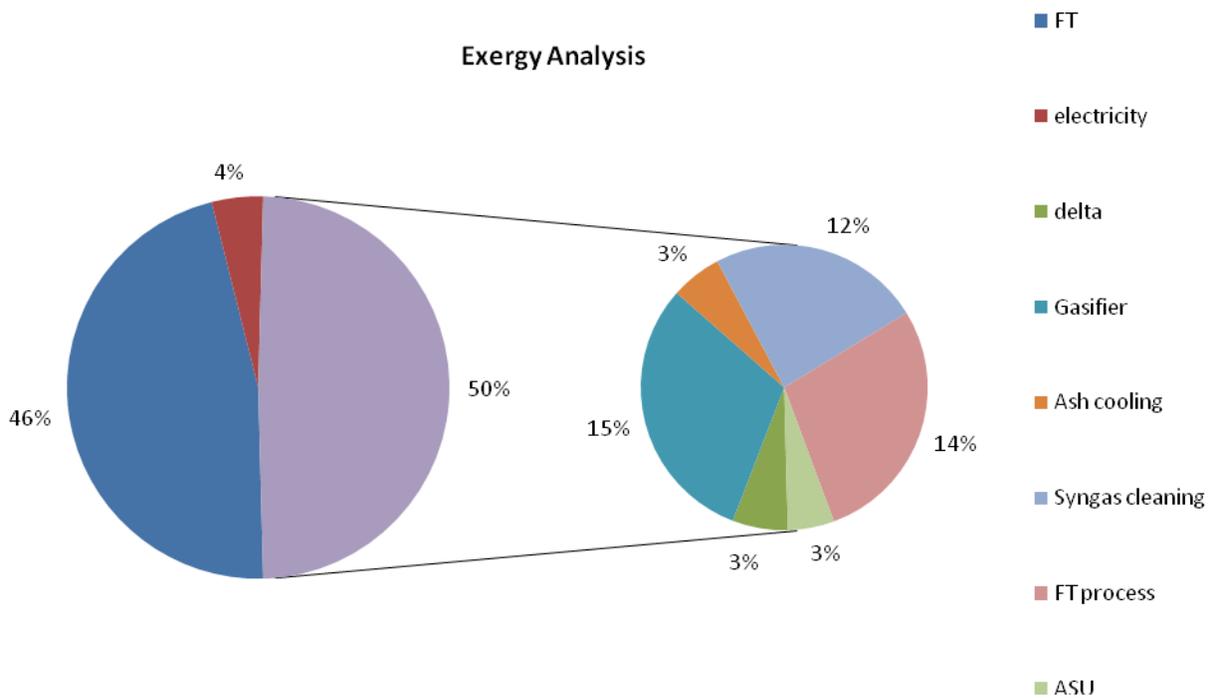


Figure 19 Exergy analysis pie-chart describing exergy losses distribution

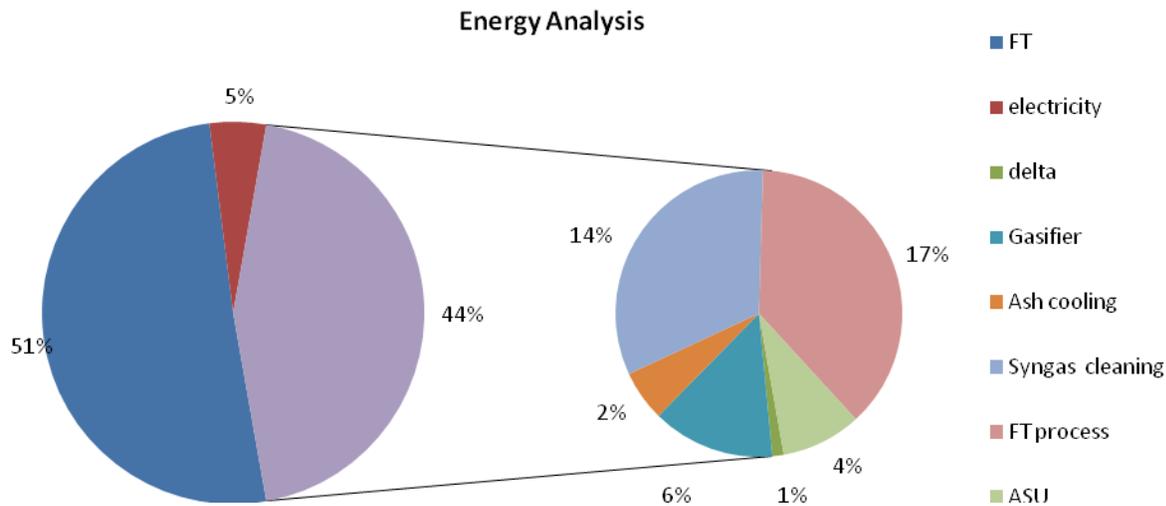


Figure 20 Energy analysis pie-chart describing exergy losses distribution

The main source of error in this approach comes from the fact that the steam produced in certain processes, like the FT synthesis and the gas cooling, is accounted here as a loss. This explains the large contribution to energy and exergy losses of these processes. A more in-depth study of the heat integration occurring in an ICL plant would certainly eliminate this problem and give a better and more realistic idea of where energy and exergy are “lost”. Even with such a large approximation it is possible to see how differently the exergy and energy losses of our system are partitioned among processes. Furthermore, in the exergy losses pie chart, the gasifier contributes to the greatest loss, as would be expected, since a solid fuel is transformed into a gaseous one through partial oxidation. This is why in the following section the gasifier is considered in more detail.

2.2.5. Energy and exergy considerations on the gasifier

From the results reported above it is clear that in an ICL plant a great exergy loss occurs in the gasifier. This is why we used the two gasifiers modeled for coal and co-firing of coal and biomass described in section 2.1 to evaluate how the performance depends on certain parameters. Again there are simplifications in the model that could be improved in a more in depth study. For example the kinetics of char combustion for coal and biomass are not included (we consider 99 % carbon conversion efficiency). Hereafter the sensitivity analysis of the gasifier on the oxygen flow and the percentage of biomass will be presented as examples. To further improve this study the model and the approach used could be used to evaluate the performance in regards to other parameters, like the temperature of the gasifier, the type of biomass and coal used, the flow of steam etc.

The parameters that were considered for this sensitivity analysis are defined as follows:

- Energy Efficiency: $= \frac{\text{Energy output}}{\text{Energy Input}}$
- Chemical Efficiency: $= \frac{\text{Chemical Energy Output}}{\text{Chemical Energy Input}}$
- Rational Efficiency: $= \frac{\text{Exergy Output}}{\text{Exergy Input}}$
- Chemical Exergy Efficiency: $= \frac{\text{Chemical Exergy Output}}{\text{Chemical Exergy Input}}$

The rational efficiency of the gasifier in the base case used for the simulation of the ICL plant is about 81% which is in good agreement with literature value of 79% [52]. Figure 21 shows the behavior of these parameters when the oxygen flow is varied between -12% and +21% from the base case.

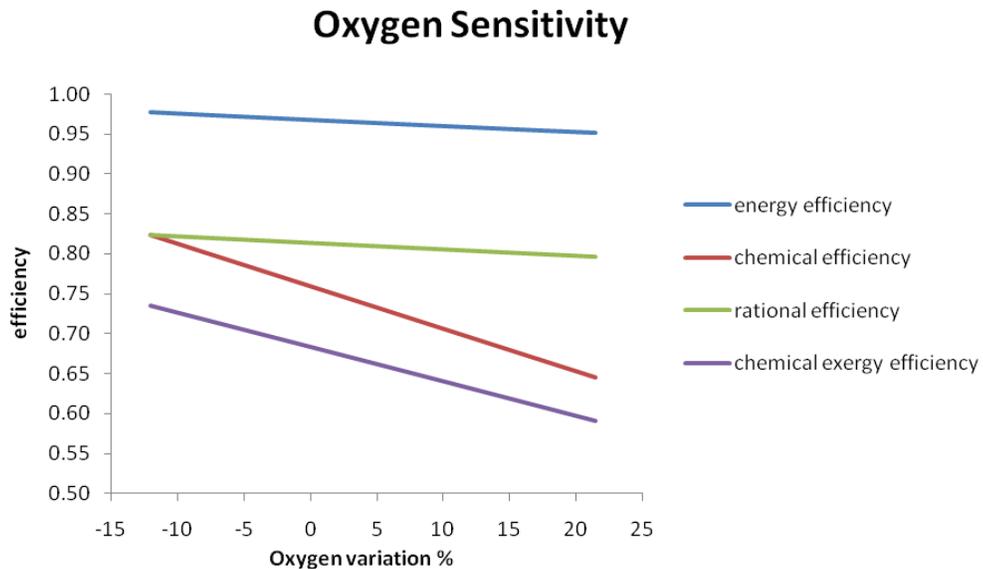


Figure 21 Oxygen sensitivity analysis

The energy efficiency, as can be seen above, does not convey much information as it is very close to one for all values of the oxygen flow which is likely for a well insulated gasifier. On the other hand, chemical, rational, and chemical exergy efficiency decline over an increasing flow of oxygen. This can be explained by the fact that as the oxygen flowrate is increased combustion takes over partial oxidation increasing the amount of heat produced at the expense of the chemical energy and exergy of the syngas. The rational efficiency considers the heat produced which explains why it does not decrease as much. On the other hand, chemical efficiency decreases more than chemical exergy efficiency because the latter also includes as an input the chemical exergy of the oxygen. Furthermore, the difference between energy and rational efficiency can be mainly attributed to the different value of the heat stream in the two cases. The energy of the heat stream was multiplied by the Carnot factor at 1600 °C (temperature of the gasifier) to obtain the corresponding value of exergy.

In Figure 22 the performance of the gasifier is evaluated as a function of the percentage of biomass, in terms of high heating value of the input, included in the feed.

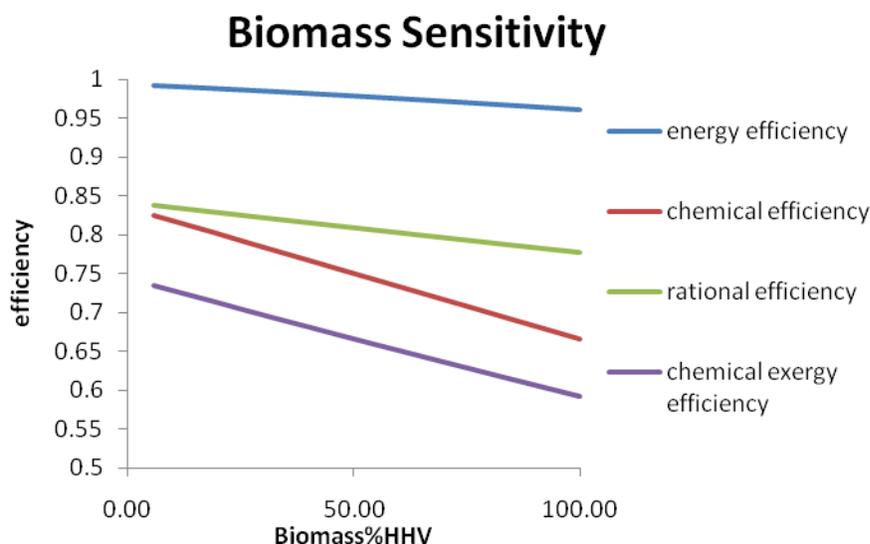


Figure 22 Biomass sensitivity analysis

The biomass sensitivity graph was obtained by varying the relative amount of biomass in respect to the coal, on a high heating value basis. The results turn out to be very similar to the one for oxygen sensitivity. This is because, as can be seen from the ultimate analysis, as the biomass input increases so does the oxygen input with the feed. In the oxygen sensitivity analysis the negative effect on the efficiency can be attributed to the excess of oxygen in the feed that leads to combustion over partial oxidation. A more detailed analysis would consider the optimal oxygen to fuel ratio for each biomass and coal combination.

2.3. Environmental Analysis

In this section the environmental impact of the ICL plant is assessed. The impact will be evaluated in terms of greenhouse gas emissions (CO₂), air quality, water usage and solid waste generated.

2.3.1. Greenhouse-gas emissions & air quality

GHG from designed ICL plant

The carbon dioxide (CO₂) emissions from the 50,000 bbl FT liquids/day plant simulated in Aspen Plus are reviewed in this section. The CO₂ generated in the plant can come from three different sources: the combustion of syngas for the production of electricity (or for raising steam quality), CO₂ generated from gasification and consequently separated in the acid gas removal process, and CO₂ generated from the FT reaction. The allocation of CO₂ from these sources is shown in Figure 23.

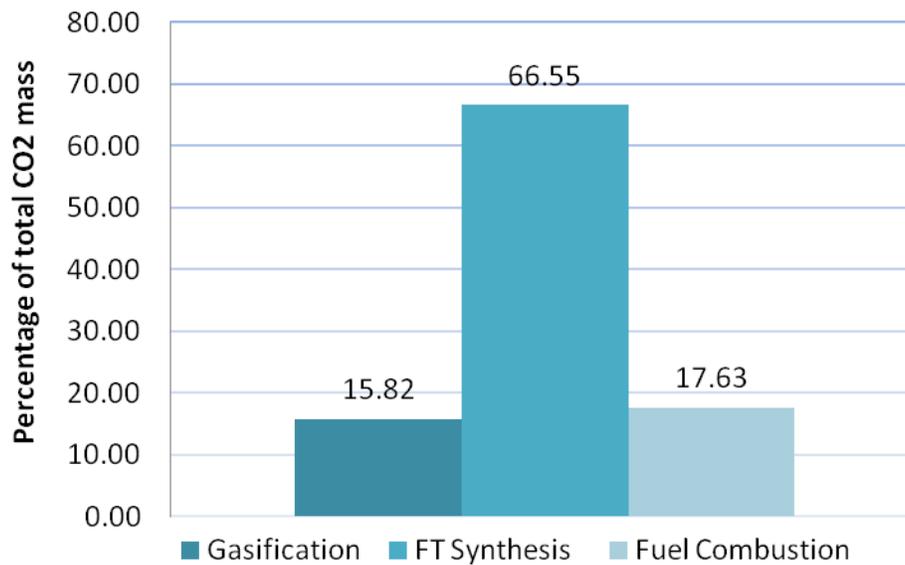


Figure 23 Sources of carbon dioxide emissions in ICL plant

As observed in the graph, a large portion of the carbon dioxide comes from the FT synthesis reactor, generated by the water-gas shift reaction that occurs in this process[53]. Ultimately, after the product is cooled, the stream originated from the FT reactor is in a mixed phase, consisting of FT liquids and residual gases that are separated by a two-phase separator producing a highly concentrated stream of CO₂. The composition of the process streams carrying the bulk of CO₂ are shown in Table 6.

Table 6 Carbon dioxide mass concentration in process streams in Aspen simulation

Simulation Stream Name	Source	CO ₂ Purity (%)
CO ₂	Gasifier – post Selexol	99
FLUGAS	FT Synthesis	95.28

The “CO₂” stream separated by the Selexol process and the “FLUGAS” from the FT reactor (post-separation) show the high purity of CO₂ in them; hence displaying the capture-ready feature of the plant design. Nevertheless, even with the possibility of storage and sequestration of the already captured CO₂ there will be emissions generated by the burning of syngas: the quality of the steam produced throughout the plant needs to be increased in order to produce electricity through a steam turbine so a fraction (12% by mass) of syngas was burned; consequently, generating extra carbon dioxide. The combusted gas stream will not have the same CO₂ concentration and readiness for sequestration as the other CO₂ streams, so it will likely be vented, unless the plant design includes a secondary capture process (Selexol, MEA, etc.) that would handle flue gas streams.

Results for the total CO₂ impact of the plant are presented in Table 7. In literature there are various forms in which CO₂ emissions are presented, so for comparison purposes the most frequent ones are shown here. Results are comparable to literature studies for 50,000 bbl/day plants. The CO₂ emissions are lower since the ICL plant modeled does not include the refining steps for the FT product, which may slightly increase the CO₂ based on extra fuel combustion for steam needs in the hydrocracking reactors and other refining steps.

Table 7 Summary of carbon dioxide emissions from ICL plant

	kg CO ₂ eq/GJ fuel	tonnes/day
From syngas production	16.28	4,405
From FT reaction	68.48	18,524
From burning syngas for elect.	18.14	4,907
Total CO₂ produced	102.90	27,836
Lit. values for same size plant	99.00[53]	28,420[54]
TOTAL CO₂ vented	18.14	4,907
TOTAL CO₂ ready for capture	84.76	22,929

GHG Emissions from Biomass-to-liquids and Co-firing

An approach to decrease the net CO₂ emissions from an ICL plant is to incorporate biomass in the feedstock. Through a combination of CCS and co-firing of biomass it is possible to reduce the total fuel-cycle CO₂ emissions to values lower than conventional petroleum fuels[53]. Different scenarios were evaluated to analyze the variations in GHG emissions by incorporating biomass. Besides 100% coal-to-liquids, a 100% biomass-to-liquids (BTL) plant and a co-firing configuration (3:1 = coal: biomass) (CBTL) were also simulated in Aspen Plus.

Figure 24 shows the different well-to-tank CO₂ emissions achieved by the simulated plants according to their feedstock composition. It is evident that 100% coal feedstock has the highest CO₂ emissions and the effect of changing 25 wt% of the feedstock to biomass is apparent by a decrease in 15 wt% of the emissions. Biomass can store close to 1,180 kg of CO₂ per ton of biomass, assuming soil and root carbon build up rate of 0.3 ton of carbon per ton of biomass over a 30 year period, and that 7% of the biomass is loss during delivery[53]; hence the net emissions of a 100% biomass-to-liquids plants could virtually help reduce CO₂ from the atmosphere, as it is shown for the BTL configuration. Results suggest that BTL would help reduce CO₂ emissions, but unfortunately studies show that the BTL industry has some limitations in terms of land availability and transportation of the feedstock so it is expected that combined solution, such as CBTL may prove to be an optimal strategy to convert indigenous coal and biomass to fuels while lowering the environmental impact of coal utilization. Comparisons of these configurations to conventional fuels and other transportations means will be presented in the comparative analysis section later in this report..

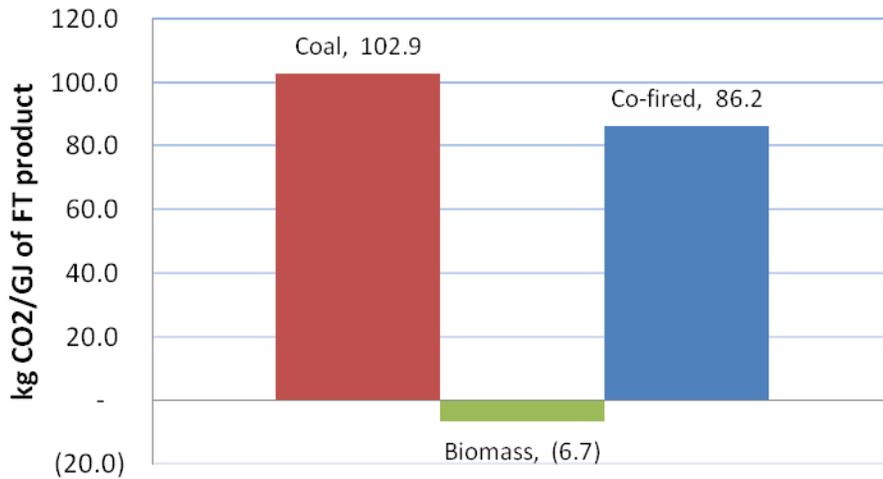


Figure 24 Well-to-tank carbon dioxide emissions from various feedstock configurations

Air quality

As shown in Table 8, the CO₂ process lines in the plant are those coming from the FT reactor (FLUEGAS) and the acid gas removal (CO₂) during syngas cleanup. The streams are highly concentrated (over 95 w%) in CO₂ and the bulk of the “impurities” mainly consist of nitrogen. The flow distribution of the impurities in the FLUGAS stream is shown in Table 6. The gasifier oxidant was 95% oxygen which explains the presence of nitrogen in the FLUGAS gas stream separated from the FT product.

Table 8 Flows for non-CO₂ gases in the FT FLUEGAS stream

Impurities in FLUGAS	Component	Flowrate (tonne/hr)
~5 w% of FLUGAS from FT reactor	N ₂	38.25
	CO	35.60
	NO	3.52E-01
	SO ₂	3.12E-05
	SO ₃	1.82E-02
	H ₂ S	8.39E-09
	COS	1.89E-02
	NH ₃	1.33E-01
		1.69E-02

Air quality concerns are probably not going to be a major setback for development of ICL in the US since the technical advances in pollution control that have been made in the past decade, mainly for power plants, allow the capture of any regulated pollutants well below environmental regulations[55]. Mercury emissions are of special concern due to the trace amounts found in coal, however, indirect coal liquefaction requires the extensive removal of

mercury and sulfur in order to protect the catalyst in the FT reactor, so it is unlikely to be an issue.

Fuel combustion may be the only source of nitrogen oxides in ICL plant and depending on the level of emissions it may be necessary to implement selective catalytic or non-catalytic reformers (SCRs and SNCRs) to keep the NO_x emissions below regulated levels. Increased efficiency and waste-heat recovery in plant designs will have an effect on the fuel needs of the plant and thus its environmental impact.

2.3.2. Water consumption

The three major requirements of water for an ICL plant come in the form of process water, boiler-feed water and cooling water. Process water is used in the actual process and sometimes is an additional component in the reactions; such is the case for the water (steam) used in the gasifiers where the water is consumed in the reaction and must be replaced. Boiler feed water is used for steam generation and the condensate is generally recovered and recycled to the boiler; that is unless the steam raised is meant to be consumed in the process. Finally, cooling water is a large requirement in ICL plants and refineries since many of the processes are highly exothermic. The “heated” cooling water is generally sent to cooling tower where evaporation of a fraction of it allows it to cool down; however, this evaporation is generally one of the factors increasing the water consumption of the plant[56].

The water and steam lines from the designed ICL plant are displayed in Figure 25. The major consumption of water is used for cooling process lines, especially for the cooling of the FT reactor and its effluent. Keeping the temperature controlled during this highly exothermic process is essential for the equilibrium of the reaction, hence close to 50% of the cooling water is used for this purpose. Syngas cooling also requires a great portion of the cooling water (30%). A lot of steam is raised from the cooling process and it is assumed a large fraction of it will be used for electricity generation, although some of it may require further heating to reach higher pressures.

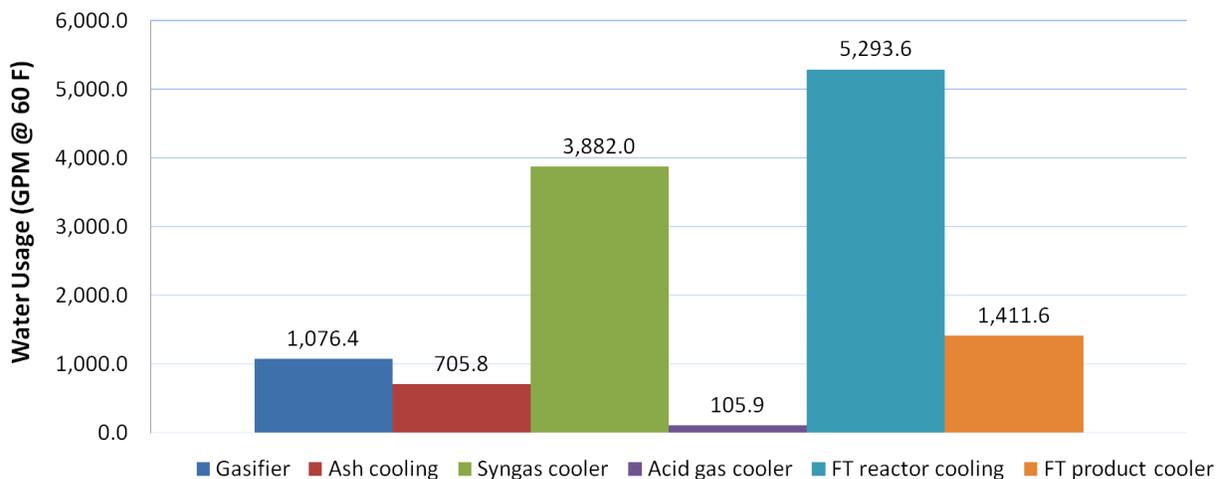


Figure 25 Allocation of water usage in the ICL plant

Generally, 97% of the cooling water is recycled and the remaining 3% is assumed lost by evaporation and must be replaced[56]. The net water consumption in the plant (replaced water) is calculated from the 3% of total cooling water and the consumed processed water by the gasifier making it a total of 1,243 gallons per minute (GPM) as presented in Table 9.

Table 9 Summary of water usage & distribution in ICL plant

	GPM	gal water/gal FT liq	Literature gal water/gal Ftliq
Water recycled in plant	11,232.0	7.70	-
Water replaced	1,243.3	0.85	1.03[53]
Total water usage in plant	12,475.29	8.55	7.30[56], 8-10[55]

Total water consumption in ICL plants will depend on various factors, including location of the plant and consequent water availability, and even properties of the local coal. Plants built in arid states like Wyoming and Montana will probably require a plant design that minimizes water usage, such as incorporating dry cooling towers, even though this technology is still not fully developed and the cost implications are highly uncertain[55]. As it has been said many times, “water may be the next oil” so the development of a ICL industry in the US will have to not only have to incorporate a technology to effectively deal with GHG emissions but also to mitigate the water consumption associated with it.

2.3.3. Waste management

The bulk mass of solid waste from the ICL plant will be generated as coal ash or slag[55]. Coal ash comes from inorganic constituents of coal, mainly silica, alumina, and smaller quantities of oxides of iron, magnesium, calcium and other elements. Ash poses concerns mainly because of metal leaching into water resources. It also contains some toxic elements in trace quantities, which depending on their concentration may sometimes demand preventive environmental management. The simulated ICL plant incorporates a slagging gasifier which melts the ash into a vitreous mass; unlike bottom ash, ash slag is less susceptible to water leaching, which makes its disposal less hazardous to groundwater resources. There has been extensive research proposing the use of gasification slag as an additive for construction materials, such as concrete or ceramics[57, 58].

Table 10 Solid waste lines from designed ICL plant

Solid waste lines	Content	Fr Equipment	Tonnes/day	kg ash-slag/bbl FT _{liq}
COOLASH	slag particulate	Gasifier Particulate	1807.8	36.71
FILTSOL	matter	filter	9.4	0.19

Table 10 shows the solid waste streams for the ICL plant. The coal used had around 10.9 wt % dry basis yields by weight. Yet, a 50000 bbl/day FT liquid plant generates ~1800 tonnes per day of ash slag that needs to be disposed of. That is equivalent to ~37 kg of ash per barrel of FT liquids produced. Hence, it is necessary that plants are constructed near landfills that have the capability to withhold this amount of waste and that will not overflow and pose damage to human health or the ecology.

Currently, there are federal and state regulations for the disposal of ash/slag from coal-power plants but there are no regulations for the disposal of slag from gasification units and even less for ICL plants. It is likely that these regulations will come into place if the ICL industry starts developing in the US, especially due to public pressure: there have been over 100 bills introduced over the past 2 years to improve the waste management of coal power plants spurred over the several ash-waste-pools that have leaked in the past [59].

2.4. Economic Analysis

An economic analysis was performed on the ICL plant based on input variables such as: financing, feedstock and product market value and escalation factors, technical design criteria, general facility parameters, and two separate contingency factors. A complete list of inputs can be found in the following methodology section. The major outputs are Net Present Value (NPV), Return on Investment (ROI), Payback Period, year-to-year “at hand” and “discounted” cash flows, a sensitivity analysis, and graphical representations of the most sensitive parameters as they relate to ROI.

A 12% discount rate was applied to the discounted cash flow in attempt to normalize the results of this study to that of DOE reports. The discount rate is applied to account for time value of money - from which ROI is directly calculated. ROI serves as a tool for investors deciding which projects to invest in. The aim of this economic analysis was to determine at what crude oil market value an indirect coal-to-liquids facility could achieve an ROI of approximately 20%- the point at which a project would move forward from being ‘technically feasible’ to ‘economically attractive’.

2.4.1. Economic Methodology

In attempt to collect the necessary input assumptions, several sources were utilized; a few are summarized in the following:

- Aspen simulation and energy analysis in order to determine thermal efficiency, coal and oxygen requirements, Fisher Tropsch product quality and distribution (ratio of diesel to naphtha), and ‘ball park’ variable maintenance costs derived from requirements such as water usage and ASU compression requirements.

- Multiple DOE and NETL reports [60] [61] [62] [63] were analyzed to determine assumptions for coal, electricity, and crude oil escalation, as well as generally accepted debt to equity ratios used for determining interest payments.
- Comparison of current market value of Ultra Low Sulfur Diesel (ULSD) vs. standard crude and a similar analysis for the Naphtha product.
- Review of related DOE reports to determine typical assumptions for commercial scale Coal-to-Liquids facility lifetimes, scaling and contingency factors, capacity utilization factors, fixed maintenance and start up costs, electrical capacity and electrical usage
- IRS 15 year Modified Accelerated Cost Recovery System (MACRS) depreciation schedule for gasification facilities [64]

2.4.2. Model Construction & Assumptions

The economic model was constructed from the ground up using an Excel Spreadsheet in order to derive a system of equations that would be specific to the project at hand. The model is designed as to be robust, intuitive, and reproducible. All base case values used are currently accepted technical, financial, and market scenarios. The market crude value was adjusted to meet an ROI of 20% prior to conduction of the sensitivity analysis.

Summary of major assumptions

- 85% Facility Availability [63]
- 30 year lifetime [63]
- 1.25 multiplier for Ultra Low Sulfur Diesel (ULSD) market value vs. petroleum crude [61]
 - FT derived diesel has ultra low sulfur, high cetane, and low aromatics
- Naphtha is valued at 77% of petroleum crude due to high degree of subsequent upgrading required. [61]
 - low octane values outweigh the low sulfur benefit
- 40% tax rate
 - 6% loan interest
 - 3% financing fee
 - 2% start-up costs
 - 55 : 45 debt to equity ratio
 - 15 year loan repayment period
- 3% escalation on market crude oil [61]
 - 2% escalation on coal and electricity
 - 2% general inflation
- 15 year MACRS depreciation schedule [64]
- Base year delivered coal value of \$42/ton [60]
 - 24,500 tons/day coal delivered
 - 12,200 BTU/lb as received
- 50,000 bbl/day FT liquids output

- 65 : 35 Diesel to Naphtha ratio for FT product
- Co-production of 290 MW electricity during normal operation
 - Saleable @ 6.0 cents/kWh
- 25% contingency factor applied to the facility reflecting uncertainty of a Pioneer design. [61]
 - Additional 25% contingency for specific FT processes due to the lack of any commercial scale utilization of FT processes in the United States [63]
 - nth plant designs (3rd or 4th of its kind) should reduce contingencies

2.4.3. Economic assumptions not included in the model

- Sulfur: 600tons / day valued at \$10/ton amount to less than 0.1% total sales [62]
- Slag – little or no saleable value, likely to be disposed of off-site or used as backfill for the supply coal mine [62, 63]
- Water Usage: Three Million gallons/day charged at \$1.5 per thousand gallons amounts to less than \$2 million per year
- CO₂ – This report has not focused on utilizing CO₂ as a saleable co-product, but rather the technical designs of constructing a ‘carbon capture ready’ facility.
 - This implies a small capital expense (that has been accounted for in the expected plant costs) for additional compressors capable of sending the CO₂ to 2200psi; typical standards for sequestration, chemical usages, and enhanced oil recovery
 - There is little to no economic incentive for CCS in the United States at this time, however, constructing a facility that is carbon capture ready will allow management to defer CCS until it may be economical to do so.

2.4.4. Sensitivity Analysis

A sensitivity analysis was performed by changing one variable at a time, $\pm 20\%$ of the base values, while holding all other inputs constant. The resulting ROI of each was plotted on a tornado diagram with the most influential parameters on top.

Table 11: Base case and Uncertainty inputs for Sensitivity Analysis

Model Inputs	Base Value	(-20%)	(+20%)
Market Crude Value (\$/bbl)	\$100	80	120
Capacity Factor (%)	85%	68.0%	100.0%
Crude Escalation (%)	3.0%	2.4%	3.6%
Project Lifetime (yrs)	30	24	36
Naphtha Value (% crude)	77%	61.6%	92.4%
ULSD Value (% crude)	125%	100%	150%
Electricity Costs (cents/kWh)	\$0.06	\$0.048	\$0.072
Coal Escalation (%)	2.0%	1.6%	2.4%
General Inflation (%)	2.0%	1.6%	2.4%
Construction Financing (%)	7%	5.6%	8.4%
Delivered Coal Price (\$/ton)	\$42	\$34	\$50
Contingency Factor (%)	25%	20%	30%
O&M Costs (%)	5.0%	4.0%	6.0%
Tax Rate (%)	40%	32%	48%
Debt to Equity Ratio (% Debt)	55%	44%	66%
Diesel to Naphtha Ratio (% diesel)	65%	52.0%	78.0%

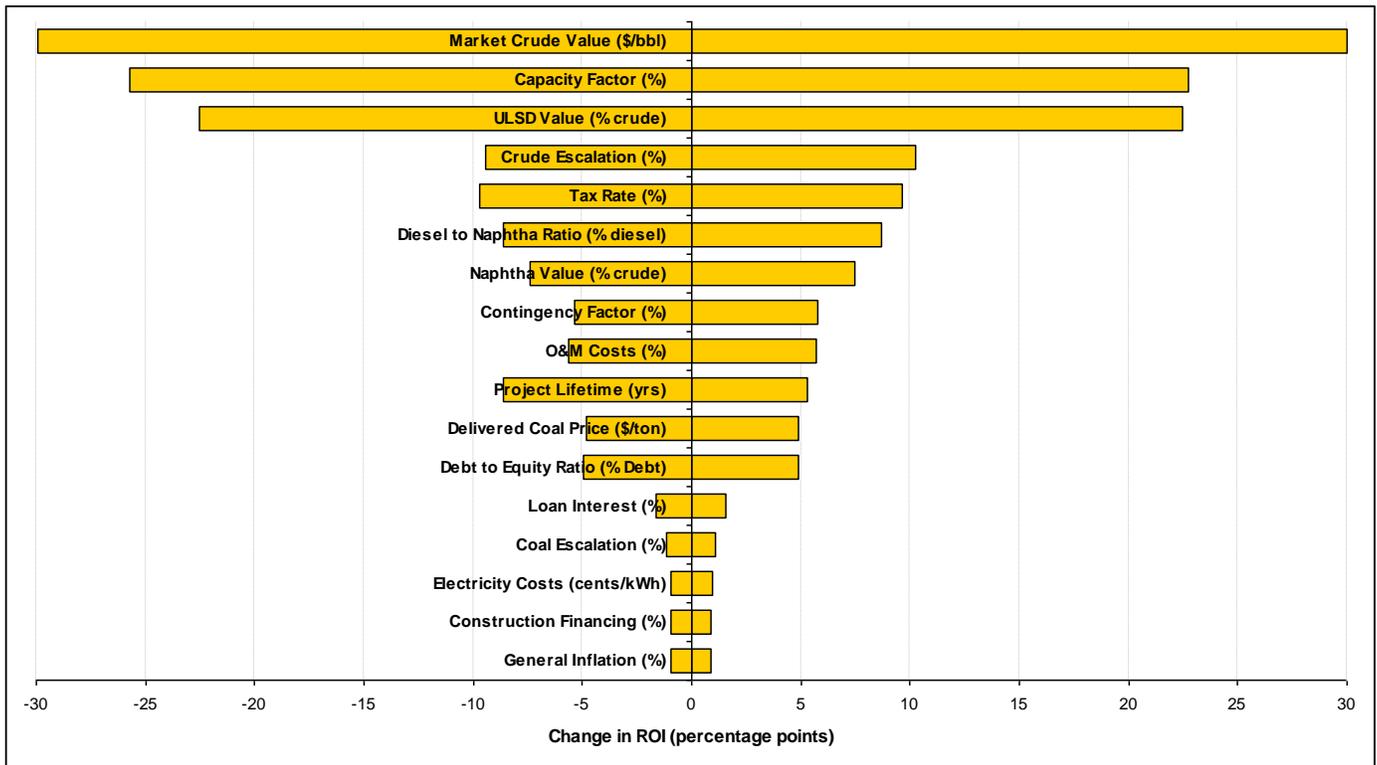


Figure 26: Tornado Diagram of Sensitivity Analysis

2.4.5. Economic Model Results

It can be concluded from this analysis that the most influential input variable effecting Return on Investment is the market selling price of crude oil. Crude selling price must reach approximately \$97/bbl in order for the proposed Coal-to-Liquids facility to achieve an ROI of 20%. The base case scenario gives a payback period of approximately 10 years, (payback period is a preliminary indication tool used by investors that does not take into consideration the time value of money).

The model was then used to perform specific individual scenarios; however, scenarios were not performed on every input variable for reasons explained here. Inputs such as: Loan interest, coal and electricity escalation, base year electricity costs, construction financing, and general inflation had less than a three percentage effect on ROI. The second set of variables not considered for individual scenarios were those of generally accepted parameters, (essentially less degree of uncertainty): Capacity factor, adjusted ULSD and naphtha values, tax rates, ratio of diesel to naphtha product, O&M costs, and delivered price of coal.

Using the model, scenarios were considered for parameters of greatest uncertainty:

- **Scenario 1:** Base Case Scenario representing the required market value of crude oil to achieve 20% ROI. The payback period was calculated from this scenario.

- **Scenario 2:** The effect of plant lifetime on required market value and ROI
- **Scenario 3:** The effect of contingency factor
- **Scenario 4:** Carbon Capture & Sequestration

Scenario 1 (below) uses the assumption of all base value parameters to determine the required market value of crude oil. The base case scenario assumes that the facility is built CCS ready; however, sequestration is being deferred until CO₂ regulation policies are in effect. Also charted is the payback period.

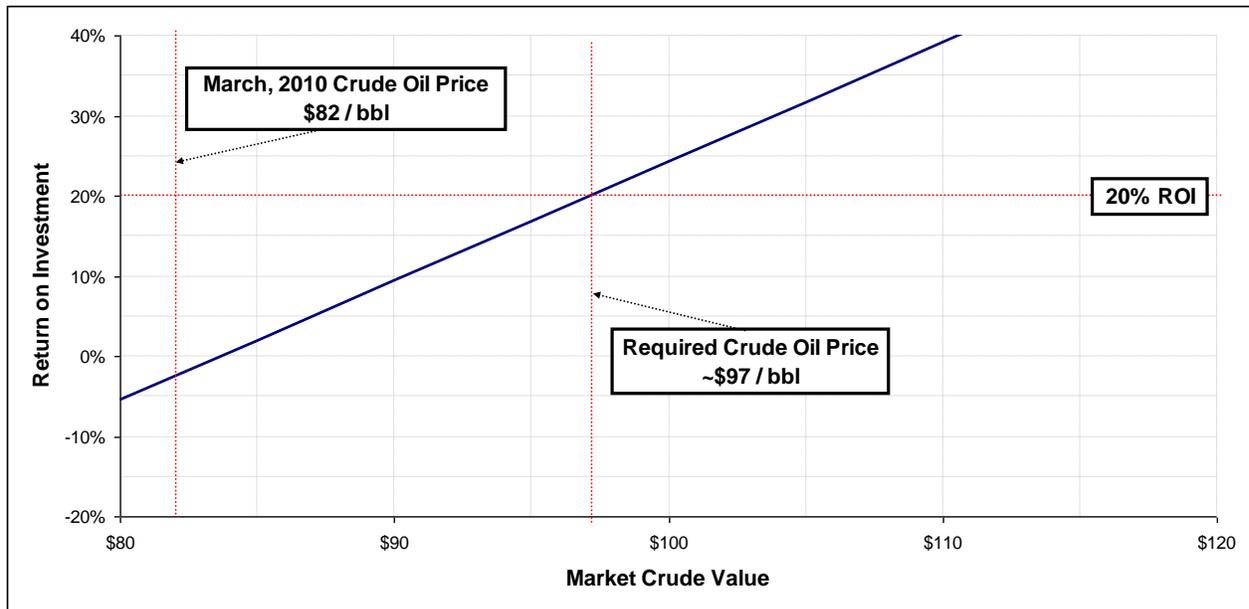


Figure 27: Effect of Market Crude Oil Value on ROI (Scenario 1)

It can be seen from the figure above that indirect coal liquefaction at this scale appears to be attractive when crude oil reaches about \$97 per barrel. As a reference point for the reader, oil is currently priced at \$82 per barrel; and at current prices positive ROI's cannot be achieved.

The graph below represents the predicted cumulative at hand cash flows. These values are not adjusted for the time value of money and are used for determining the payback period of a project. Due to the large capital expense (~ \$5.5 Billion) the payback period is perhaps longer than desired. The payback period could be reduced to 8 years if the plant is considered to be of nth design (reduced capital cost due to reduced contingency).

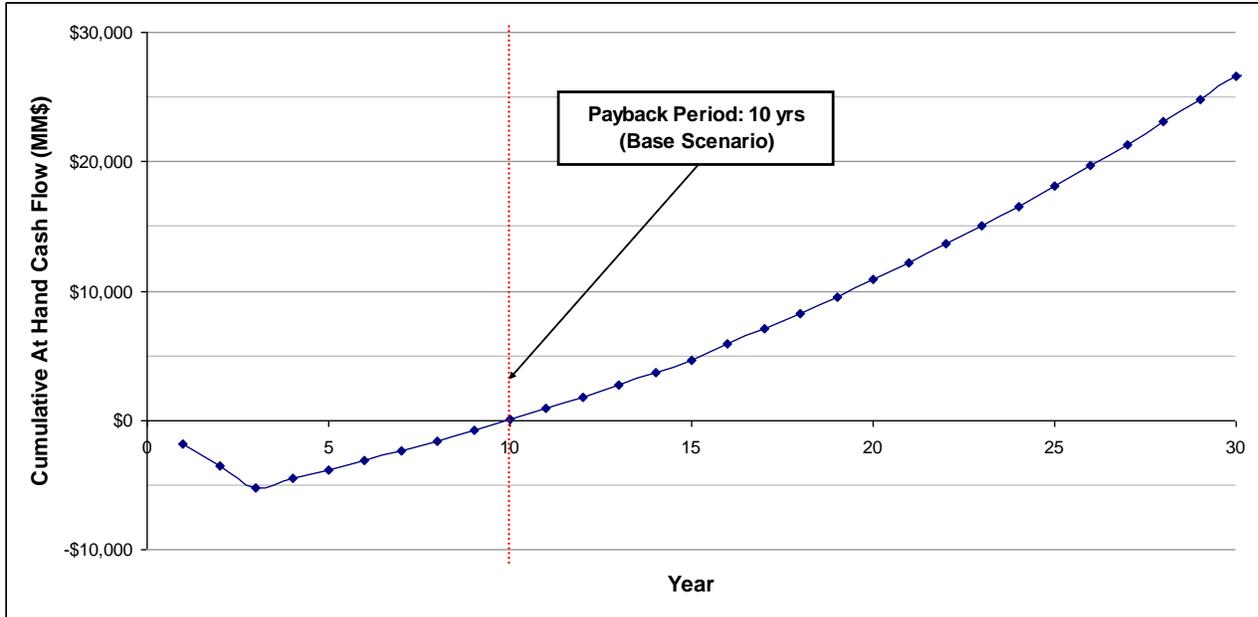


Figure 28: Payback Period (from Base Case Scenario)

Scenario 2 (below) examines the effect of altering plant lifetimes. It should be noted that due to the inherent nature of applying discount rates, the lifetime of the plant will have a stronger negative impact when adjusting the plant lifetime the same number of years shorter vs. longer; the effect is seen in below. It is shown that a 36 year lifetime would require a base year market value of \$94/bbl; while the assumption of a 24 year lifetime would require \$103/bbl to meet the same ROI value.

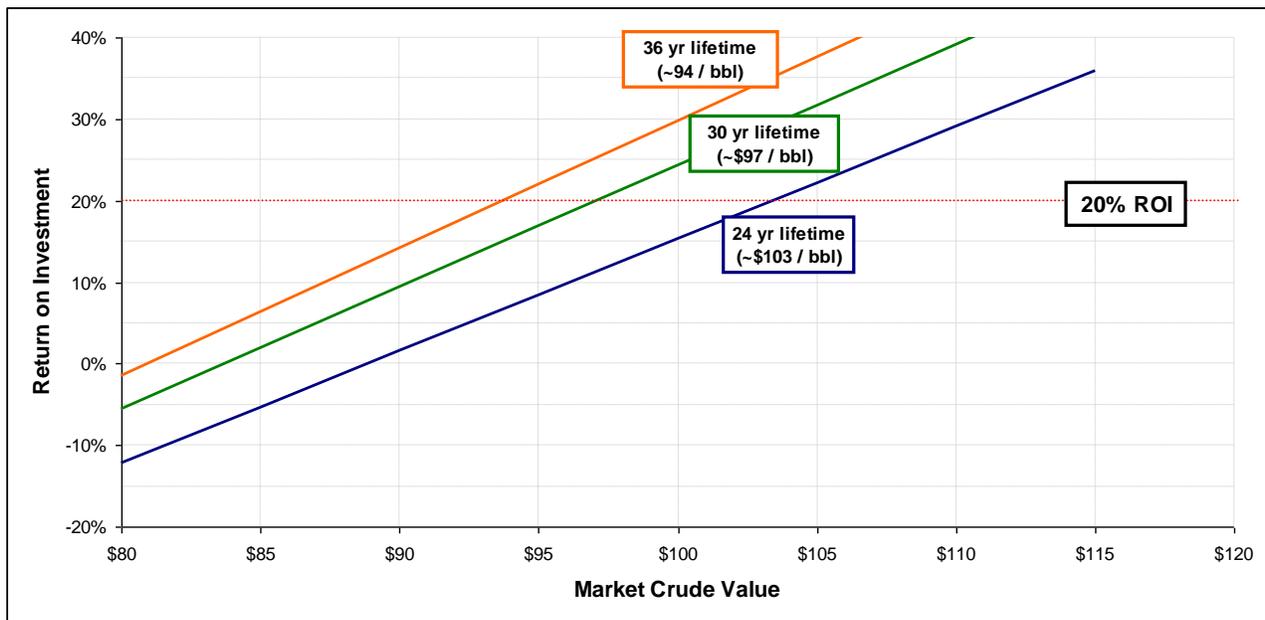


Figure 29: Effect of Plant Lifetime (Scenario 2)

The next scenario analyzed involves contingency factors and takes into account capital cost uncertainties of pioneer plants vs. a plant of n^{th} design (3^{rd} or 4^{th} of its kind). If the assumption of an n^{th} plant is made it is likely that the contingency factors would be reduced, or even eliminated. In this scenario, the contingency values are reduced to 10%, (from 25% base value)

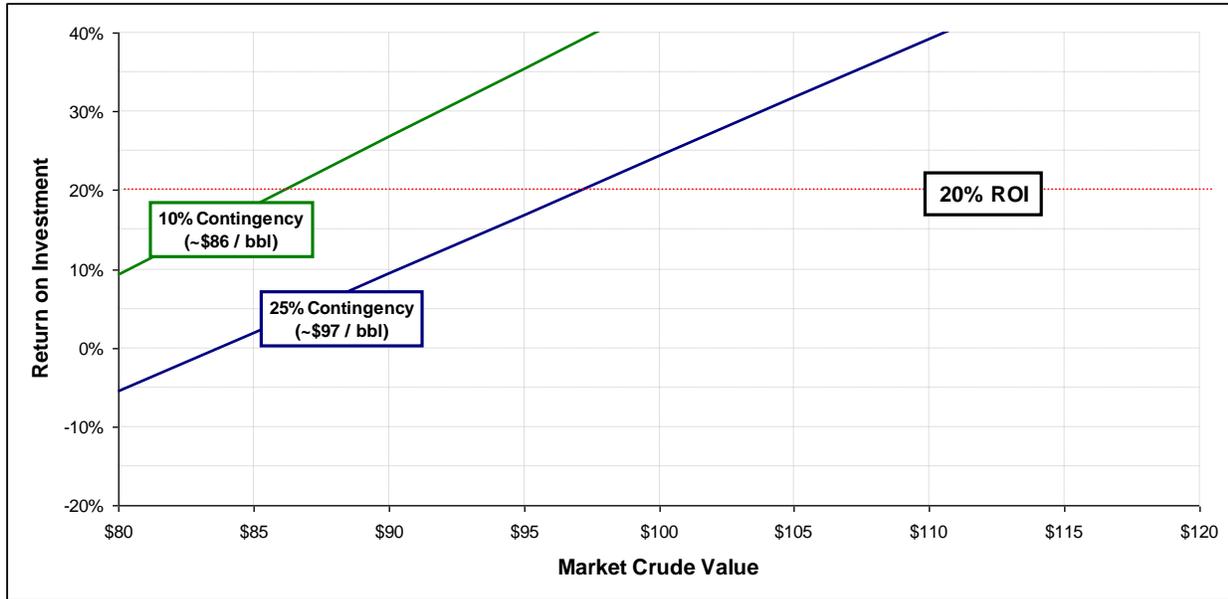


Figure 30: Effect of Contingency Factor (Scenario 3)

With these assumptions in place, the required market crude oil price is reduced from \$97/bbl to \$86/bbl. This indicates that, in the future after a few commercial scale CTL facilities have been constructed, it may become increasingly profitable to produce Fischer Tropsch liquid fuels from coal.

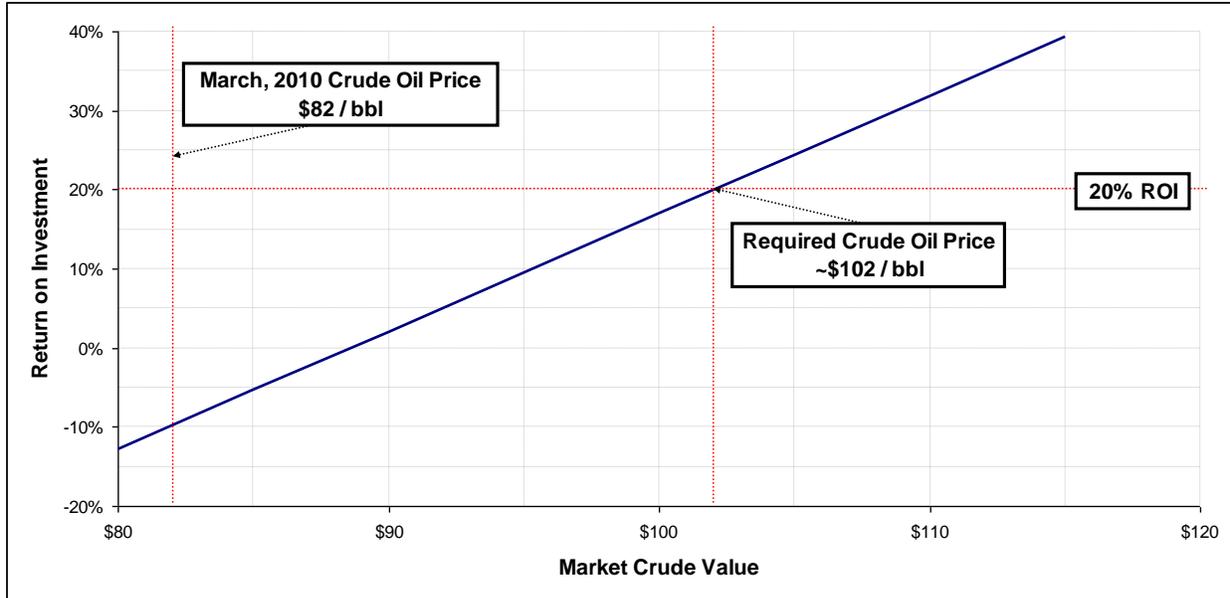


Figure 31: Effect of Capture and Sequestration (Scenario 4)

As mentioned before, all scenarios have included a carbon capture ready facility. Scenario 4 (above) assumes that the facility is actively capturing and sequestering CO₂. The added costs include \$7 / ton to compress and transport CO₂. The pipeline distance from the reference Dakota SNG plant is 200 miles and the pressure requirement is assumed to be 2200 psi. It can be seen that the required selling price to meet the same ROI is increased from \$97 to \$102/bbl.

2.4.6. Possible Future Work

An opportunity for future work exists in altering the specific ratio of poly generation capabilities of the Coal-to-Liquids plant. This study assumes that part of the syngas is burned to raise high quality steam to produce electricity. This generally provides just enough power to run the facility during startup which leaves 290 MW available during normal operation to be sold to the grid. Firing more than just the off-gas syngas from the FT reactor would allow for additional electric capacity; however, detailed analysis would be required to determine the coal, oxygen, and overall thermal efficiency changes. In addition, capital costs are likely to increase with added electrical generation capacity.

While the focus of this study has not been on direct coal liquefaction, possibly of interest is the quality of gasoline and diesel produced from indirect and direct coal liquefaction. FT diesel (the indirect pathway) is the primary component (65%) of the simulated ICL facility and is low in sulfur and aromatics and has a good cetane[65] rating; unfortunately, the United States consumes much more gasoline than diesel. The gasoline produced from the naphtha product is generally lower quality: low aromatics resulting in a low octane number. The direct coal to liquids pathway produces exact opposite results, good gasoline and less desirable diesel[66]. Direct coal liquefaction is only being practiced on a commercial scale at one facility worldwide (in Mongolia) for a number of reasons, namely related to the high degree of maintenance

associated with DCL. In direct liquefaction coal is crushed and mixed in hydrogen rich slurry at 350-400°C. As physical chemistry dictates, gas is less soluble in liquids with increasing temperature; therefore, in order to keep the hydrogen in the mixture, pressures upwards of 2000 psi are required. The pressure let down of the three-phase flow between the reactor and the solid/liquid separation unit has the effect of sandblasting through the valve, subsequently resulting in valve lifetimes less than 30 hours.

Because direct liquefaction requires hydrogen anyway (similar to an ICL plant), a gasifier is a likely addition to the facility which gives rise to the potential of merging the two technologies. If DCL produces desirable gasoline and ICL produces desirable diesel, a combination of the two technologies in one facility would be ideal for producing high quality and quantity liquid transportation fuels. It is, conceptually, a simple matter of running two different water gas shift reactors. The first would produce the H₂/CO ratio desired for the FT reactors and the second would shift the process entirely to hydrogen for the direct liquefaction hydrogen requirements.

2.5. Policy prospects for ICL

The future commercial development of ICL in the US will significantly be affected on the extent to which the federal government provides incentives or disincentives for private early investment in ICL projects[65]. In addition, the course of development of ICL will be bound to existing and forthcoming environmental regulations that comprise greenhouse emissions, land, water and biological impacts. These issues are discussed in the following section.

2.5.1. Federal Policy Prospects

There are three different positions the federal government can adopt with regards to ICL and other unconventional liquid fuels. It could assume a hands-off policy and allow the marketplace to decide whether or not to develop an ICL industry and how to do so, while supporting R&D that does not involve large investments such as non-demonstration activities and long-term technologies. This is basically the position the federal government has taken since the 1990s where most, if not all, ICL projects that spurred during the late 1970s were terminated due to the drop of crude oil prices [65, 67]. On the other hand, the government may choose to actively promote the development of a commercial ICL industry by providing subsidies and other incentives to enhance the competitiveness of fuels from unconventional sources such as ICL. It is expected however, that the government would take a middle position between these two extremes such that both the private and public sector can be benefited.

The main factor presently holding back federal government support for ICL development is the consequent environmental impacts associated with ICL processes linked to increase in coal mining activities and greenhouse gas emissions. The United States has yet to develop legislations for this issue, in the meantime, uncertainty as to when and how these regulations will work continues to hinder the investments from private sectors.

2.5.2. Barriers

2.5.2.1. Remaining Uncertainties

The prospects for developing an technically viable ICL industry in the United States are promising; however important uncertainties have delayed private investments [65], such as

- Uncertainties about the production costs of ICL.
- Uncertainties about the future of crude oil prices, chances that coal liquids may not be cost-competitive with petroleum-derived fuels.
- Uncertainties about future regulations of greenhouse emissions.

The one that appears to have the most weight on the private sector investments is the uncertainty about crude oil prices. The large financial investment required by ICL facilities is one that not many firms can bear. The possibility that oil prices may fall significantly during the life of an ICL project, especially during the initial construction stage, increases the financial risk in an appreciable manner driving away many investors. The main concerns for investors are in regards to extremely low rates of return or even project bankruptcy due to inability to pay back debts.

2.5.2.2. Carbon Dioxide Control Policies

There is an international consensus that mitigation of greenhouse-gas emissions and the slowing of climate change will only be achieved when industrialized nations establish a regulatory framework that would put a price on emitted carbon dioxide and other greenhouse gases, either through a market-based mechanism such as carbon tax or cap & trade, or through a direct regulation. It is only through economical penalties or rewards that industries and consumers will be pushed to improve the technology and manners of using fossil energy. Unlike Europe, there are currently no binding regulations at the federal level to reduce carbon dioxide emissions in the US. Numerous climate-related legislative proposals that include cap-and-trade systems have been introduced for the past four years, never coming to fruition due to lack of consensus in congress. A bill introduced last year known as the American Clean Energy and Security Act of 2009 has been passed in the House and will follow to be voted on in the Senate[68].

Basically, the bill discusses issues such as the creation of clean energy jobs, achieving energy independence, reduction of GHG emissions and transition to a clean energy economy. In terms of GHG emissions, it proposes the establishment of a cap-and-trade system and setting goals for reducing such emissions from specified sources by 83% of 2005 levels by 2050[68]. Depending on the intricacies of this regulation, this could represent a barrier for the near-time development of ICL while CCS technologies remain immature in the US. The establishment of this bill may remove some of the uncertainties holding back the investment on ICL projects. Nonetheless, without CCS policy incentives, the US government will unlikely support the development of a ICL industry large enough to reduce the dependency on foreign oil [67, 69].

Because of the emerging relevance of carbon mitigation, the development of an ICL industry in the US is closely tied to the feasibility of carbon capture and storage operations. Apart from technical, geological and geographical issues still remaining with CCS, there is still no specific regulatory framework for carbon storage. So far, it is covered by the Federal Underground Injection Control (UIC) Programme under the Safe Water Drinking Act which regulates the injection of hazardous and un-hazardous materials[67]. The American Clean Energy and Security Act of 2009 addresses key legal, regulatory barriers to the deployment of commercial-scale carbon capture and sequestration. It is the lack of regulations, as explained before, that generates uncertainties and will keep these issues as barriers until these deficiencies are solved.

2.5.3. Incentives for ICL

Major petrochemical companies are likely the most suitable firms to develop of substantially large ICL projects, since they possess the technical and financial resources to embark on these multibillion dollar projects. It is up to the government to create financial mechanisms that would encourage the involvement of these companies as well as other capable ones. This can be achieved by the generation of policy incentives for investments from the private sector. Some of these are:

2.5.3.1. Subsidies

It has been discussed[65, 67] that investment subsidies in the form of *investment tax credits* and accelerated depreciation are a good option for raising private after-tax internal rate of returns, regardless of the status of economical uncertainties such as the crude oil price. Despite what the crude oil price is, tax credits can financially help the investor from the beginning of the project (construction stages) at the expense of the government.

Another type of possible subsidies is *production subsidies*, which would benefit the usage of unconventional fuels as opposed to conventional-petroleum fuels. These may work through the extension of the tax credit that currently supports alcohol fuels (corn ethanol) to unconventional fuels, for instance. Nonetheless, this type of subsidy functions as a fuel credit, which makes it the least cost-efficient for the government and could negatively impact the federal budget [65]. Moreover, this approach discourages energy conservation and increasing efficiency in energy use.

Before September of 2009, there was a subsidy of this type known as Alternative Fuel Tax Credit which established a volumetric excise tax credit of 50 US cents per gallon (13 US cents/l) for alternative fuels used in motor vehicles, including coal liquids derived through the Fischer–Tropsch process [67]. However, the credit was limited until September 30th 2009 and has not been extended since then, perhaps for the reasons explained above.

An opposite approach to a subsidy that may work in favor of ICL production is the application of a petroleum tax that would increase the price of conventional petro-fuels only. This approach would supposedly recognize the value and efficiency of the individual choices of consumers and producers. The concept is apparently not new, but has mainly been used to promote the usage of some type of petro-fuels over another (LPG vs. gasoline in the Netherlands and China) [65, 70, 71]; but since this policy involves the raise of transportation fuel prices, it is often seen as a dangerous political move by the occupant government and therefore disregarded.

2.5.3.2. Price Floors & Income Sharing

Price floors are a government- or group-imposed lower limit to ensure prices stay high so that products can continue to be made. This financial instrument could encourage private investment for ICL by removing the uncertainty of financial constraints in the case that the price of crude oil happens to go below the economical threshold. Price floors would allow the increase of the real after-tax internal return of investment [65] during times when average oil price is low. Moreover, this instrument is not so disadvantageous for the government since it implies no cost to the government during times when the average oil price is high enough.

Conversely, there is also a policy that can be beneficial for the government to recover the public funds associated with these means of promoting early investment of ICL, known as income-sharing. When oil prices are high and ICL investors are financially healthy, in exchange for a government-set price floor or any other subsidies, the investor may pay the government a portion of its net income when, after taxes, it is sufficiently large to keep the financial viability of the project. Basically, it is like a setting a pay-back time/scenario for the government to recuperate from the support given for the development of the ICL industry causing the least financial harm possible for them. A balanced combination of these financial instruments (price floor, an investment tax credit and an income sharing agreement) could be a policy package to promote private investment on ICL in a nearby future even while the United States still relays on imported oil [65].

PART 3: COMPARISON OF ICL TO OTHER CRUDE OIL ALTERNATIVES

It would be nice to think of the future of United State's transportation as a minimal polluting infrastructure with highly efficient emission-free vehicles. Unfortunately this future is far away. Some say that with the soon "end of oil"[72] vehicles will transform into cleaner machines, and others claim that oil comes from a "bottomless well"[73]. If the US does lose its current oil imports, whether by science or by politics, what can be done to keep the transportation sector alive without an enormous environmental or economic hit? There are three main types of fossil fuels: crude oil, natural gas and coal. If crude oil is taken out of the picture, natural gas and coal could help fill in the gap.

Natural gas (NG) is a common fuel for many applications, but currently NG is not a common light duty vehicle fuel in the US. As a transportation fuel natural gas can be compressed and

used directly as a fuel, it can be gasified to form syngas for an F-T reactor to produce either synthetic diesel or gasoline, it can also be used to produce methanol or dimethyl ether (DME). Natural gas contains a high elemental ratio of hydrogen and can be used for fuel cell vehicles, the natural gas can be reformed for pure hydrogen vehicles, and natural gas can be used as an electricity prime mover for electric cars. All of these natural gas options are being researched for their transportation potentials.

In the United States the majority of our fossil fuel energy content is from coal. Coal, similarly to natural gas, can also be used as a feedstock for hydrogen and electricity production for fuel cell or electric cars. However, coal can also be used in coal liquefaction processes: direct and indirect, as described earlier in the report. Indirect liquefaction processes, like the one analyzed in this report can produce high quality diesel fuel for our transportation fleet.

Besides fossil fuel sources, alternative transportation fuels in the United States could be produced by renewable sources. Wind turbines can produce the electricity for electric car batteries, solar panels can produce the energy for splitting water to produce hydrogen for fuel cell vehicles, and biomass can be transformed into hydrocarbon fuels for internal combustion engines. This section of our report compares our detailed indirect coal liquefaction plant to these other alternative transportation options.

3.1. Methodology

Two different initial approaches were used in comparing transportation fuel options. A large literature search was conducted to find reliable and comparable data in energy, economic and environmental categories. This search led to some contrasting values; different literature bases their results off different assumptions. As a group, we used our background knowledge to sort through the available numbers and by comparisons and calculations, chose which sources were the most relevant to our work. This unfortunately is an inherent limitation of our data which contributes to the uncertainty of our analysis. A system was created to normalize these results and transform them to the most unbiased comparisons as possible. For example, a fuel cell vehicle could claim to be more powerful than an electric vehicle; however this may be because the power capability of the fuel cell is higher than that of the battery. To normalize this, a power rating of 80kWe was set for both electric and fuel cell vehicles' motors. Similarly normalization was chosen for gaseous fuels' pressure to be consistently calculated at 200bar and all coal processes were set to use the Illinois No. 6 coal just as with our indirect liquefaction plant. Below is the list alternative fuels compared along with their nomenclature.

- Petroleum diesel @ \$100/barrel of crude oil (Petro diesel)
- Petroleum gasoline @ \$100/barrel of crude oil (Petro gas)
- Biodiesel soy and woody biomass (B100)

- Ethanol from corn (E85 corn)
- Ethanol from switchgrass (E85 SG)
- Compresses natural gas, 200bar (CNG)
- Synthetic natural gas from IGCC, 200bar (SNG)
- Hydrogen from NG internal combustion at 200bar (H2 NG ICE)
- Hydrogen from NG in a 80kW fuel cell vehicle, 200bar (H2 NG FCV)
- Hydrogen from wind energy in 80kW fuel cell vehicle, 200bar (H2 WE FCV)
- Electricity from fossil fuels in a 80kW electric vehicle (FF BEV)
- Electricity from photovoltaic energy in a 80kW electric vehicle (PV BEV)

The problem statement of this study clearly states that we will analyze an indirect coal liquefaction plant in the case that the United States no longer has reliable crude oil sources, but for the point of interest, we have included petroleum gasoline and diesel fuels in these literature comparisons.

The second method of analysis, other than literature sources, was by use of The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model[74]. The GREET model is free software developed by Argonne National Laboratories sponsored by the Energy Efficiency and Renewable Energy (EERE) department that can analyze transportation fuels for energy values and CO₂ emissions. The inputs of this software allow variables to be selected on nine of our desired comparative fuels and were consistently kept to calculations on passenger cars for the 2010 year:

- Gasoline vehicle (Petro gas)
- Diesel vehicle (Petro diesel)
- Dedicated CNGV (CNG)
- EtOH; fuel flexible vehicle: E85, Corn (E85 corn)
- Hydrogen vehicle; internal combustion engine. hydrogen from NG (H2 NG ICE)
- FT diesel; from gasification of coal (ICL diesel)
- Biodiesel from woody biomass (B100)
- Electric car; from US elec. mix (FF BEV)
- Hydrogen vehicle; fuel cell. Hydrogen from NG (H2 NG FCV)

The outputs of the GREET model are simplified to units of Btu/mile for energy and grams/mile for CO₂ results. From here further calculations were needed for our comparisons. This particular software does not address economics.

3.2. Energy

Quantitative energy comparisons are predominantly broken into two categories: the energy to produce the transportation fuel, referred to as “well-to-tank” and the energy used in the vehicle operation is referred to as “tank-to-wheel.” Other energy considerations, including energy to produce the feedstock and energy needed to produce raw materials or equipment, will be covered later in this report. In Table 12 the efficiency of the fuel production is listed. These efficiencies only include the energy of the feedstock (i.e. woody biomass, crude oil) and the energy of the fuel. The energy density for the end product fuels are listed in Table 13 below.

Table 12: Fuel production efficiency

WELL-TO-TANK	
Fuel alternative source	Well-to-tank efficiency
ICL diesel	51.3%[75]
IBL diesel	50.8%[75]
Petro diesel	82%[74]
Petro gas	82%[74]
B100	36%[74]
E85 corn	45%[74, 76]
E85 SG	28%[76]
SNG	40%[77]
CNG	87%[74]
H2 NG ICE	58%[74]
Hydrogen and electricity production for FCV and BEVs	
H2 NG FC	58%[74]
H2 WE FC	35%[74]
PV BEV	15%[74]
FF BEV	27%[74]

Table 13: Fuel energy density

ENERGY DENSITY	
Fuel	LHV (MJ/KG)
Synthetic diesel	44.6[75]
Diesel	43[78]
Bio-diesel (B100)	37[78]
Gasoline	43[78]
Ethanol (E85)	29[78]
CNG (200bar)	45[78]
Hydrogen (200bar)	120[78]

Well-to-tank efficiency does not include the energy it takes to produce the feedstock. These values are significantly important when it comes to the energy to produce bio-fuels. Crop production energy requirements in decreasing order for corn, soy, and switchgrass are roughly 9,450 kWh/hectare, 4,350 kWh/hectare, and 3,200 kWh/hectare[76]. This points out that even though corn to E85 contains the highest well-to-tank conversion of the biofuels, near that of our ICL plant, the feedstock production energy requirements cannot be ignored when considering the overall process and would inevitably lower this efficiency in comparison. In Figure 32 this energy production well-to-tank efficiency is compared to the fuels tank-to-wheel lower heating value and fuel economy[79].

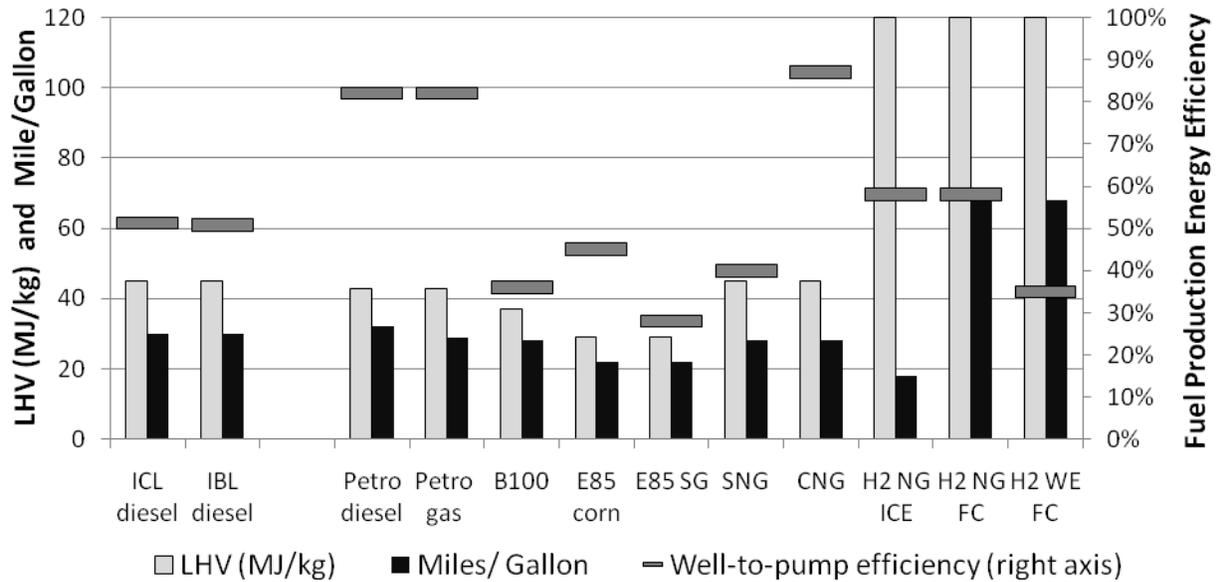


Figure 32: Well-to-tank and tank-to wheel fuel comparisons. Battery electric vehicles contain no values for lower heating values.

As seen in Figure 32, comparing our designed indirect coal to liquid plant to other alternative fuel production facilities places our facility (~51%) a bit above average (~44%) for well-to-tank production efficiency. It must be noted that the Aspen Plus simulation plant efficiency is considering all outputs as diesel, where in fact some of this product is not high enough grade diesel and will require refining from the local refinery. For battery electric vehicles (BEVs) containing an 80kWe motor the fuel economy is around 1.5 miles/gallon gasoline equivalent (GGE = 120MJ) for a 35% efficient vehicle (some vehicles claim 75% efficiency[79]) this was calculated from current electric car data[80, 81]. Some new hydrogen I.C.E. pick-up trucks tested by the government are showing 27miles/gal[82].

In energy comparisons, ICL synthetic diesel contains a higher energy density than other liquid alternative transportation fuels and shows a better fuel economy. Compared to gaseous and electric transportation fueling options, these liquid fuels are difficult to compare. As for well-to-tank production efficiencies, compressed natural gas and hydrogen production from natural gas are more efficient than the ICL plant in this form of comparison. Natural gas and hydrogen alternatives are efficient in production and about on par in fuel economy. On an energy-basis-only these technologies are very competitive if not superior to indirect coal liquefaction.

3.3. Environmental

Environmental considerations are of both quantitative and qualitative forms. As discussed in the prior part of this report, the Aspen Plus modeled indirect coal liquefaction plant has the potential to release large amounts of CO₂. And it was also shown how this can be reduced with the addition of biomass fuel mixing. Figure 33 shows how this modeled plant's CO₂ emissions compare to the other alternative transportation fuels as calculated from the GREET modeling software.

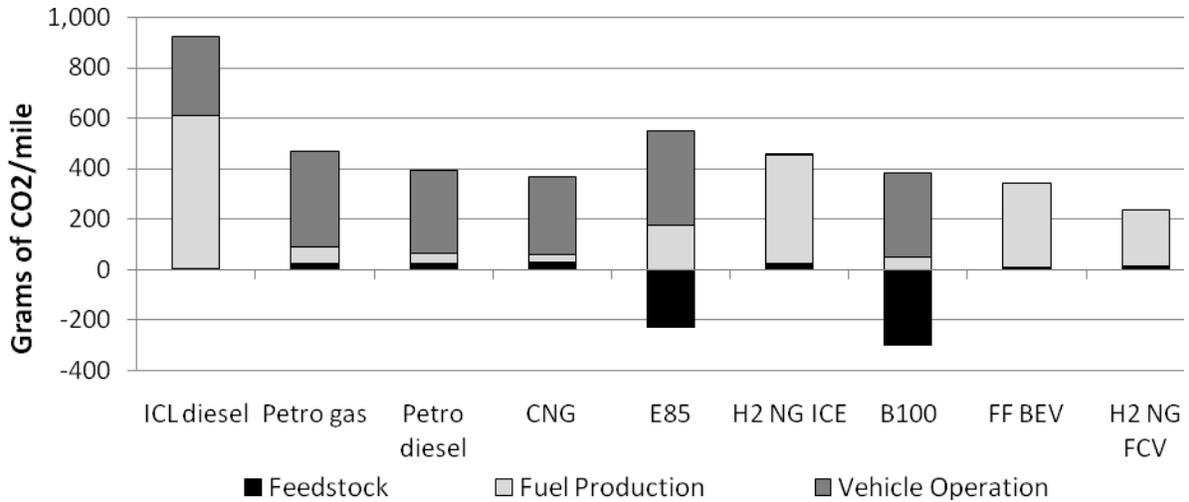


Figure 33: CO2/ mile GREET model outputs

The GREET model is the ideal way to show these results over literature because it keeps the numbers in the most consistent form possible. Some CO₂ data from literature is shown in Figure 34. Here data is shown in grams of CO₂ per MJ: how much CO₂ is emitted from producing a MJ of the fuel and how much CO₂ is emitted from utilizing a MJ of the fuel in the vehicle.

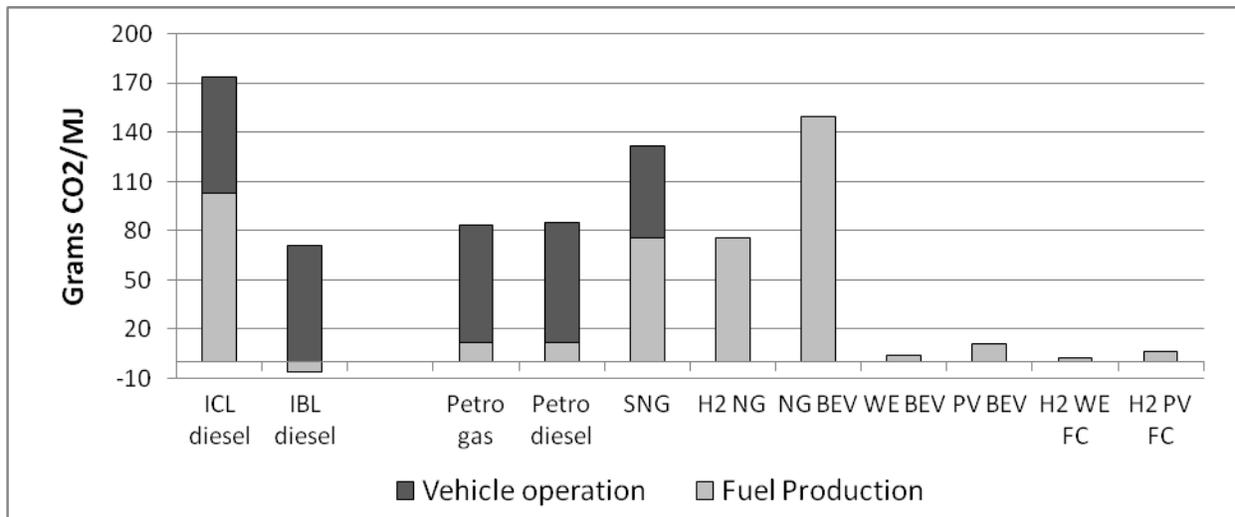


Figure 34: CO2/MJ literature[77],[78],[83] and Aspen Plus[75] values

These two graphs clearly show a large disadvantage of producing synthetic fuel by means of indirect coal liquefaction. If the ICL plant uses only coal as a feedstock and no carbon capture and sequestration, renewable energy sources, like wind energy and photovoltaic electricity are far superior when comparing CO₂ emissions from fuel production. But, CO₂ emission is not the only environmental concern to compare with other alternatives.

Biofuels may look promising: B100 production not only releases low net amounts of CO₂, but B100 compared to petro diesel and synthetic diesel exhausts lower particulate matter, carbon monoxide, and hydrocarbons, and it is less toxic and safer to handle according to the EPA. On the other hand, B100 in vehicle operation increases nitric oxide (NO_x) production, a precursor to acid rain, ground ozone, and deforestation[84]. Also, as with all biofuels, large amounts of land must be consumed for fuel feedstock. In one report it is stated that “wrecking land for biodiesel results in higher CO₂ emissions than the use of fossil fuels,”[85] and in another it is stated that “40 acres of land produces only enough energy for a vehicle to travel 20 miles”[86] Biofuels have long been under attack for their use of land and water resources so changing our synthetic fuel input from coal to biomass might just change the environmental concerns, rather than solve them.

Emissions from hydrogen and electric vehicles are near null, but if these fuels are produced from fossil fuels their production emissions cannot be ignored. One kg of hydrogen production from steam reforming (considered a gallon equivalent) emits a total of 11,900 grams of CO₂, methane, and nitrous oxide_[87]. Electricity production from natural gas produces about 20,000 grams of CO₂ per gallon equivalent (33.4kWh, 120MJ) along with nitrogen oxide emissions, dependent on emission control technologies. This CO₂ per energy value of fossil fuel electricity emissions (167 gCO₂/MJ for NG BEV) are very near that of the total ICL figures which includes the CO₂ emitted from diesel combustion (174 gCO₂/MJ total for ICL diesel). This answers the very commonly asked question: even though electric vehicles emit no exhaust, if the electricity is from fossil fuel power without CCS, there is no CO₂ emission advantage. Renewable energy fuel production is not yet environmentally perfect either; electric cars running on electricity produced from solar PV are dangerous in their requirements for mining of precious metals. Additionally the production of batteries and fuel cells can contain hazardous materials and utilize industrial facilities that require energy, water, and dangerous chemical disposals. Depending on the specifics of individual facilities these issues can be minor or major.

3.4. Economics

A detailed economic analysis has been discussed for our domestic indirect liquefaction in a previous section of this report. This section will discuss economics in much simpler terms as to compare ICL to the other crude oil alternatives. The break even selling price for FT derived crude oil is approximately \$2.07 per gallon. This breakeven price yields an ROI of 0% over the facility lifetime (30 years). Current prices for fuels in the state of Illinois are shown in Table 14. All of these values were obtained from soliciting fuel stations, except the compressed natural gas price was obtained from cngprices.com, and hydrogen citations are located next to the sale price values. It should be assumed that the pump price of ICL diesel will be the same as Petro diesel.

Table 14: Current sale prices for fuels in Illinois

FUEL	Sale Price (IL)	Units
ICL diesel	3.00	\$/gallon
Petro diesel	2.99	\$/gallon
Petro gas	2.77	\$/gallon
B100	3.67	\$/gallon
E85	2.19	\$/gallon
CNG	1.80	\$/gallon
H2 NG	3.30 ^[88] ^[89]	\$/kg
H2 WE (est.)	5.50 ^[88]	\$/kg
FF electric	0.08	\$/kwh
PV electric	0.32	\$/kwh

Electricity is a cheap fuel on the market for the consumer, but this fuel price does not consider the fact that a battery electric vehicle (BEV) costs an additional \$10,000 more than an average car with an internal combustion engine^[90]. A fuel cell vehicle can cost around \$3,500-\$4,000 more depending on the fuel cell stack^{[88],[90]}. From current car markets an 80kWe motor can require about \$3.00 to fill which will last 100 miles^[80]. Synthetic fuel from an ICL plant would cost a little over \$10/100miles. Figure 35 compares these along with the other studied alternatives. To normalize these values, no hybrid vehicles are included in this study, however it should be understood that vehicles' fuel economy increases by about a third when a hybrid electric system is added which in turn decreases the price it costs to drive 100 miles while increasing the initial price of the vehicle.

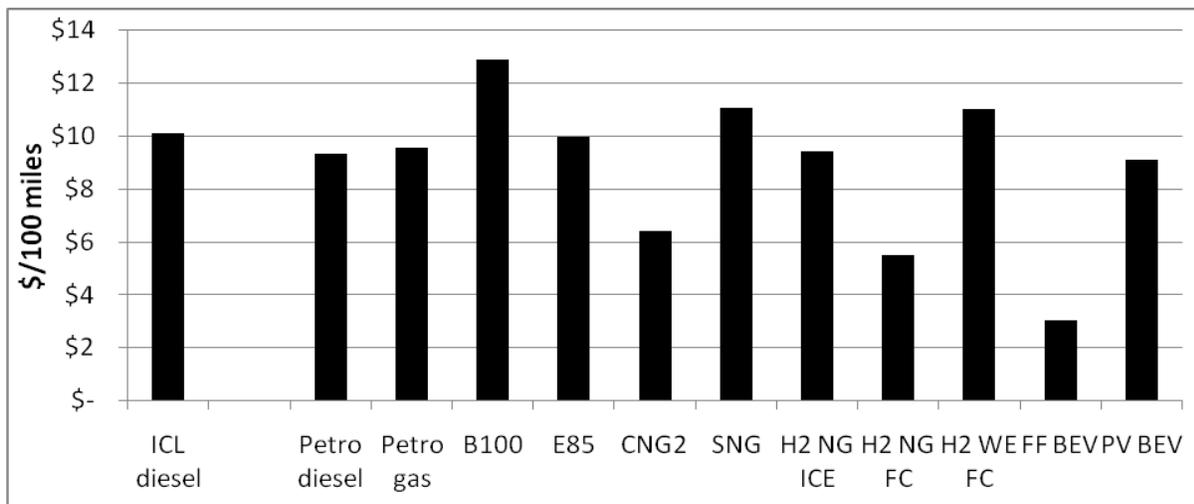


Figure 35 Fuel cost per 100 miles - tank-to-wheel

In terms of economics indirect liquefaction fuel price is one of the more expensive fuels to purchase by a very small margin, but the initial cost of the vehicle will not have to increase and this is an important factor. Maybe when newer alternative technologies are improved and mass produced, this will no longer be the case, but in the meantime paying \$10,000 more for an electric car is an issue.

3.5. Other Issues and discussion

Besides standard energy, environmental and economic comparisons, other issues must be considered, for example: safety. The gaseous hydrogen and natural gas fuels are often stored



Figure 36: Ford hydrogen I.C.E. prototype storage cells

at 200 bar. The new proposed Ford hydrogen ICE vehicle is planned to run on hydrogen stored at 345 bar, and even then it only stores enough hydrogen for 200 miles of driving between fills. Not only are these high pressures, but the gases are flammable (as meant to be, of course). Car accidents are common incidents and people do not always have all their attention at fueling stations when filling up their tanks. These issues have long been discussed and safety precautions have been installed, such as upgrading heavy steel tanks to aluminum coated with carbon fibers[91]. These tanks also take up considerable amounts of space within the vehicle[88]. Whether or not these are worthy concerns, public opinion is an unavoidable aspect of the

market.

Public opinion is also an extremely large issue with indirect liquefaction facilities like the one modeled here for Illinois. “Not in my back yard” is a common way of putting it. There is currently no existing full-scale indirect coal liquefaction to synthetic fuel facility in the United States, but the United States is still importing crude oil at less than 97 \$/barrel, this report’s calculated necessary price with a ROI of 20%. If this less expensive source of crude oil is lost, indirect liquefaction plants may overcome protest, as it produces transportation fuels with comparatively low transportation infrastructure changes.

In energy, environmental and economic comparisons natural gas and renewable hydrogen and electricity alternatives are cleaner and more efficient fuels. As for public opinion and the future of transportation fuels, there are two ways to look at this: If the environment is the biggest concern, electric, fuel cell, or ICE hydrogen vehicles could be the answer to the end of oil, provided that electricity or hydrogen are obtained from renewable resources. If change is the public’s biggest concern, then synthetic fuels from indirect liquefaction could be the easiest transition with the economic and energy advantages over biodiesel (and ethanol if considering land and resource use), and with carbon capture and sequestration, this solution would come closer to meeting both parties’ credentials.

CONCLUSIONS

The goal for this project was to evaluate indirect coal liquefaction as an alternative to crude oil and compare it to other promising transportation alternatives for the United States. This was done by carrying out a detailed Aspen Plus simulation of an ICL plant operating on Illinois No. 6 coal. The plant was envisaged to be located in Roxana, IL on the basis of different factors such as the presence of a local refinery which could upgrade the syncrude to commercial fuel. The data obtained from the Aspen Plus simulation was used to carry out both an energy and exergy analysis of the process. Through the Aspen model it was also possible to assess the environmental impact of such a plant in terms of CO₂ emissions, water consumption and waste production. In this context a detailed economic analysis was done and the issues related to policies were analyzed. Finally, to address the gist of the matter, a thorough comparison of alternative transportation technologies for light duty vehicles was carried out, relying both on literature data and on software calculations. Hereafter a brief summary of the results obtained throughout this study is outlined.

The plant was modeled to produce 50,000 bbl/day of FT diesel and generate electricity that would meet the plant needs. The coal feed rate is 2400 tonnes/hr for each gasifier. To produce the total desired plant output, eight of such gasifiers would be required. The calculated efficiency of the plant is 51.2%. This calculated efficiency does not take into account the refining of the FT diesel and the syngas cleanup section which was modeled as an ideal process. A sensitivity analysis was performed and the optimum oxygen and steam flowrate was determined to be 23.8 kg/s and 7.2 kg/s respectively. Biomass gasification was simulated and it was found that even though the net CO₂ emissions for biomass were lower, the mass of biomass that needs to be gasified to produce the same amount of FT liquids as a coal fired gasifier was almost double. Co-firing of coal and biomass at 3:1 ratio by weight was also simulated. There was not much of a difference in the energy efficiency. This might be because the milling and grinding energy losses were not taken into account.

The accuracy and depth of the energy and exergy analysis inevitably clashed with the approximations and limitations of the data available. One of the main issues was the lack of information on process heat integration that resulted in inflated losses relative to the FT reactor and gas cooling. Further approximations were necessary for ease of calculation, like considering gases (a part from steam) as ideal and standard conditions for the reference environment. Nevertheless the major energy and exergy fluxes were identified and it was possible to see how differently energy and exergy losses are partitioned throughout the plant. The exergy analysis identified the gasifier as the main source of exergy loss while from an energy point of view the gasifier's losses are negligible. This exergy loss is intrinsic to the gasification process as the breakup of the large molecules of coal (and biomass) into smaller ones inevitably results in an increase in entropy. A closer look was therefore given to the gasifier and its performance was evaluated under varying conditions, such as oxygen flow rate and biomass to coal concentration. Further work could be carried out in this direction by improving the model of the gasifier to include issues such as char behavior and detailed gasifier conditions (turbulence, heat losses etc.). A more in-depth model of the whole plant would

enable a specific assessment of where exergy losses occur and how they could be reduced. Calculations could also be carried out directly through Aspen Plus using software such as ExerCom [92] which was not available for this study. Part of the exergy losses could be minimized applying for example pinch analysis to identify the minimum heat requirement for each process and evaluate how much heat could be internally recovered [93].

The environmental impact of the modeled ICL plant was evaluated based on the results obtained through the process simulation. From this, results suggest a significant environmental concern associated with the technology is the level of carbon dioxide emissions generated by the process, which as presented in the comparative analysis, is much larger than for any other transportation alternative. It was observed, however, that part of the emissions could be mitigated by the co-firing of coal and biomass, and the CO₂ capture-readiness associated to the process is one step closer to solving this issue once the sequestration technology is economically available. Future federal policies for GHG may play a barrier for the commercial development of ICL, although the creation of CCS policy incentives may prove in favor of this technology. It is recognized then, that the development of an ICL industry in the US will be largely bound to the technical feasibility of CCS and the prospective policies associated to it.

In the economical analysis, it was observed that the crude oil market price was the main input affecting the ROI; hence, various scenarios with different economic factors were analyzed. Scenario 1 was the base case which calculates the value crude oil would need to reach in order for an indirect coal to liquids facility to be considered economically attractive. The value was determined to be ~\$97/bbl which can be compared to the current oil price of \$82/bbl. This also yields a payback period of ten years. The second scenario, regarding plant lifetimes, returned required crude oil values of \$94 and \$102/bbl for 36 year and 24 year lifetimes, respectively. When the effect of contingencies are considered, (reduced from 25% to 10%), the required crude oil selling price is reduced to \$86/bbl. Lastly, if it is decided to actively capture and sequester CO₂, the required selling price of crude oil is increased to \$102/bbl.

Indirect coal liquefaction ideal production efficiency at about 50% is lower than that of crude oil at about 82%, but compared to other alternative fuels, this efficiency is above average. Biodiesel, ethanol, electricity (from any source), and hydrogen from wind power are here found to be less efficient, and compressed natural gas from natural gas fossil fuel sources is the most efficient. As for CO₂ emissions, ICL surpasses all the other fuels, with a close total emission value to that of electricity on an energy basis. ICL does not use as much land or water as biomass sources, but if the CO₂ emissions are reduced by co-firing, this may not be the case. The economics of diesel from ICL, as discussed, are highly dependent on many outside variables. A strategic advantage of ICL is that the automobile industry and fueling infrastructure would only require small changes (gasoline-to-diesel). On the other hand replacing one fossil fuel with another may only be a temporary solution to a never ending problem, and a large infrastructure change may be inevitable.

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APPENDIX A. Location Selection

Table 15 Status of CTL Projects in the US (Source: Coal to liquids by Gordon R Couch)

Table 07 CTL plants under consideration in the USA (based on Miller, 2007)						
Project lead group	Partners	Location	Feedstock	Capacity, bb/d	Estimated cost, US\$ billion	Status
DKRW	Rentech (for FT) GE ExxonMobil (for MTG)	Medicine Bow, WY	bituminous coal	18,800	2.75*	design (2013) construction due in 2009
Rentech	KEC WorleyParsons	East Dubuque, IL	bituminous coal (converting a gas fed fertiliser plant)	1,800	0.8	feasibility (2010)
WMPI	Shell, Sasol, US DOE	Gilberton, PA	anthracite waste (culm)	5,000	0.6	design
American Clean Coal Fuels	none cited	Oakland, IL	bituminous coal (Illinois Herrin No 6) plus biomass	30,000	NK	feasibility
Alaska IDEA	Alaska NRTL CPC	Beluga Cook Inlet, AK	subbituminous coal	80,000	5 to 8	feasibility
Peabody/ Rentech	NK	MT	subbituminous coal/lignite	10,000–30,000	NK	feasibility
Peabody/ Rentech	NK	southern IL southwest IN western KY	bituminous	10,000–30,000	NK	feasibility
Rentech	Adams County	Natchez, MS	coal/petcoke	10,000	0.65– 0.75	feasibility
Baard Energy	CEC	Wellsville, OH	subbituminous coal/biomass	35,000–50,000	4	feasibility
Mingo County, WV	Rentech	Mingo County, WV	bituminous	20,000 (10,000–30,000)	2	feasibility
Synfuels Inc	GE, Haldor-Topsoe, NACC, ExxonMobil	Ascension Parish, LA	lignite	NK	5	feasibility
Headwaters	Hopi Tribe	AZ	bituminous	10,000–50,000	NK	feasibility
Headwaters (American Lignite Energy)	NACC, GRE, Falkirk Mining	ND	lignite	40,000	3.6	feasibility
NK	not known/not available					
DKRW	DKRW Energy LLC (Management team: Doyle, Kelly, Ramm and White)					
Alaska IDEA	Alaska Industrial Development and Export Authority					
Alaska NRTL	Alaska Natural Resources to Liquids					
CEC	Civil and Environmental Consultants, Pittsburgh, PA					
NACC	North American Coal Corporation					
GRE	Great River Energy					
KEC	Kiewit Energy Company					
*	EIA (2006b)					

APPENDIX C. The assumptions and kinetic parameters for the FT model

The basic assumptions made for the FT reactor were the following [31]:

- steady-state operation;
- isothermal conditions;
- large-bubble flow in plug-flow regime due to its velocity;
- assumption of hydrocarbon products in the gas and liquid phases to be in equilibrium at the reactor outlet;
- negligible mass and heat transfer resistances between the catalyst and the liquid;
- location of the gas-liquid mass transfer limitation in the liquid phase;
- Intrinsic kinetics for the FT and WGS reactions.

Table 16 Kinetic parameters for WGS and FTS in iron catalyst [42]

k_{FTS}	0.1106 (mol/kg.s.Mpa)
A	3.016
k_{WGS}	0.0292 (mol/kg.s)
K_1	85.81
K_2	3.07