

# Coal Gasification

## Final Report

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## **Executive Summary**

The main objective of this project is to design a plant which produces 5000 metric tons per day of AA methanol grade purity from coal through the process of coal gasification. The different steps involved in the process include the coal selection, coal gasification, acid removal, water gas shift reaction, methanol synthesis, and finally the methanol refinement. Montana Sub-Bituminous was chosen for the coal feedstock. The two stage dry feed entrained flow reactor, CCP gasifier was our chosen gasifier technology. The Rectisol process was chosen as our acid removal process. The Claus process was chosen as our waste sulfur treatment. The Claus process ultimately produces elemental sulfur. The water gas shift reactor must be designed to change the ratio of  $H_2:CO_2$  to 2:1. An isothermal water gas shift reactor was chosen because the reaction is highly dependent on the temperature. Thirteen plug flow reactors were used to simulate the methanol synthesis process, however this is unrealistic. The thirteen plug flow reactors produces 5143.10 tonnes of methanol per day. The distillate from the distillation column had a weight composition of 1.34% water, 98.10% methanol, 0.56% ethanol. Total profits for the 5<sup>th</sup> year are -\$1,390,524,848.00. The plant will never be profitable and the internal rate of return cannot be calculated.

## **Overall Project Scope Description**

The rapid rise of the price of crude oil and the increase in demand for chemical feedstocks has stimulated world wide investigations for alternative energy sources and chemical feedstocks. For this purpose, the production of methanol from US coal deposits has been presented as an alternative energy source from the US abundance of coal reserves. The US has an estimated 265 billion tons in coal reserves.

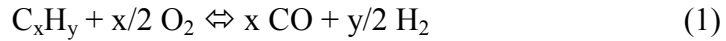
Worldwide, there is  $984 \times 10^9$  tons of coal. Coal consumption has been relatively stable for the past ten years and plays an important role in the long term energy strategies due to the abundance of coal compared to other resources. If consumption continues at current rates, the world's reserves of coal will last approximately 216 years. This is a huge difference from natural gas reserves which would last about 62 years and only 40 years for oil. Clearly, the abundance and availability of coal makes it such a promising alternative energy source over natural gas or oil.

Coal gasification refers to a process that breaks down coal into its components, by subjecting it to high pressure and high temperature in addition to the use of steam and oxygen. This leads to the production of synthesis gas, which is mainly a mixture containing of carbon monoxide and hydrogen.

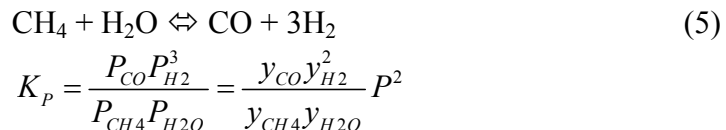
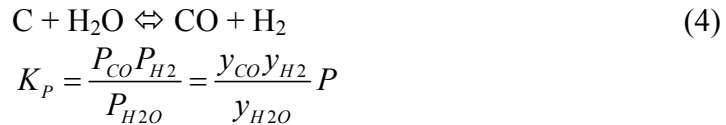
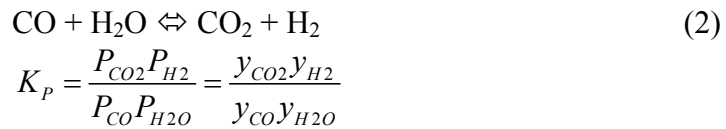
The Asia-Pacific region, specifically China, has seen a recent surge in economic growth. This in turn has seen the rise in the demand for alternate energy sources and chemical feedstocks. Coal gasification can be utilized to produce methanol as alternative energy source.

However, the production of methanol from coal is not that simple. Coal contains many other compounds and impurities that would interfere with the methanol synthesis process. Coal often contains such compounds as nitrogen, sulfur, ash, oxygen and water. Before coal can be gasified, it must first be dried. Then afterwards the coal can be gasified to produce syngas.

Coal gasification can be represented by the following reaction:



The variables x and y represent the actual composition of the coal. The following set of reactions can be used to model equilibrium reactors operating at high temperatures (in excess of 1500 °F):



Assuming these reactions are at thermodynamic equilibrium, the reactions and equilibrium constant equations provide a basis to calculate the relative concentrations of the gasifier product gas.

One important aspect of preparing the syngas for methanol production is the removal of acid gas, which can be composed of H<sub>2</sub>S and CO<sub>2</sub>. Then ideally, the syngas mixture would have a 1:2 CO to H<sub>2</sub> ratio for methanol synthesis. This is not always the case. To remedy this, steam can be used to produce more hydrogen by reacting it with carbon monoxide via the water-gas shift reaction:

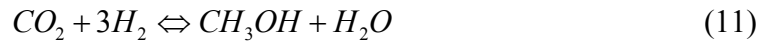


$$\ln K_p = \ln \frac{P_{\text{CO}_2} P_{\text{H}_2}}{P_{\text{CO}} P_{\text{H}_2\text{O}}} = \ln \frac{y_{\text{CO}_2} y_{\text{H}_2}}{y_{\text{CO}} y_{\text{H}_2\text{O}}} = -4.33 + \frac{4577.8}{T(K)} \quad (7)$$

From this, methanol can be produced from carbon monoxide and hydrogen via the methanol synthesis reaction:



$$\ln K_p (1/\text{psia}^2) = \ln \frac{P_{\text{CH}_3\text{OH}}}{P_{\text{CO}} P_{\text{H}_2}^2} = \ln \frac{y_{\text{CH}_3\text{OH}}}{y_{\text{CO}} y_{\text{H}_2}^2} \frac{1}{P^2} = -32.918 + \frac{11284}{T(K)} \quad (9)$$



The reaction kinetics of methanol synthesis can be modeled by the following rate equations:

$$r'_{\text{CH}_3\text{OH},A3} = \frac{k'_{ps,A3} K_{co} [f_{\text{CO}} f_{\text{H}_2}^{3/2} - f_{\text{CH}_3\text{OH}} / (f_{\text{H}_2}^{1/2} K_{p1}^0)]}{(1 + K_{\text{CO}} f_{\text{CO}} + K_{\text{CO}_2} f_{\text{CO}_2}) [f_{\text{H}_2}^{1/2} + (K_{\text{H}_2\text{O}} / K_{\text{H}_2}^{1/2}) f_{\text{H}_2\text{O}}]} \quad (12)$$

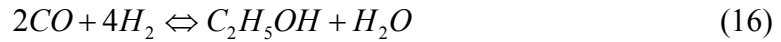
$$r'_{\text{H}_2\text{O},B2} = \frac{k'_{ps,B2} K_{co_2} (f_{\text{CO}_2} f_{\text{H}_2} - f_{\text{H}_2\text{O}} f_{\text{CO}} / K_{p2}^0)}{(1 + K_{\text{CO}} f_{\text{CO}} + K_{\text{CO}_2} f_{\text{CO}_2}) [f_{\text{H}_2}^{1/2} + (K_{\text{H}_2\text{O}} / K_{\text{H}_2}^{1/2}) f_{\text{H}_2\text{O}}]} \quad (13)$$

$$r'_{CH_3OH,C3} = \frac{k'_{ps,C3} K_{CO_2} [f_{CO_2} f_{H_2}^{3/2} - f_{CH_3OH} f_{H_2O} / (f_{H_2}^{3/2} K_{p3}^0)]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) [f_{H_2}^{1/2} + (K_{H_2O} / K_{H_2}^{1/2}) f_{H_2O}]}$$
 (14)

The values for the kinetic factors and driving force and adsorption coefficients are derived from the experimental values. To define these values, experimentally defined values for constants A and B are used in conjunction with the following relation:

$$Parameter = A \exp\left(\frac{B}{RT}\right)$$
 (15)

The syngas can also react to produce ethanol. It was assumed that ethanol is produced at a rate of 1 part per 100 parts of methanol produced (mole basis). The reaction for ethanol is as follows:



### **Design Basis, Principles and Limitations**

The whole project was designed to producing 5000 metric tons of methanol a day. The entrained flow gasifier was designed as a equilibrium reactor which minimized the Gibbs free energy. The output of the gasifier was designed to maximize the amount of carbon monoxide (CO) and hydrogen (H<sub>2</sub>) and the achieve the closest ratio of H<sub>2</sub>/CO to 2 as possible. The output of the gasifier was modified by changing the temperature, pressure and flows of the input oxygen and steam. The basis of design of the water gas shift reactor was to achieve the 2:1 ratio of H<sub>2</sub> to CO. The water gas shift reactor was designed as an isothermal equilibrium reactor with a 50 °F approach to equilibrium. The basis of design for the methanol synthesis reactors was to produce 5000 metric tons of methanol a day. The methanol synthesis reactors were modeled as adiabatic plug flow reactors (PFR) with the specified reaction kinetics. The PFRs were designed with a 50 °F approach temperature to equilibrium as well. The extent of reaction along the PFR to achieve the desired temperature and methanol production was varied by changing the amount of catalyst.

The limitations of the project is has to do with our limited knowledge of Aspen and the design of similar projects. It was unrealistic to model our reactors to handle the

total of 7500 metric tons of coal a day in a single gasifier or water gas shift reactor. Also the number of PFRs and amount catalyst were unrealistic (13 PFRs and ~500 metric tons of catalyst used).

### **Technology Selection Criteria and Conclusions**

#### *Choice of Coal*

The first step in the process of coal gasification is the selection of an appropriate coal. The available sources of coal were analyzed and compared in terms of their costs and compositions, which included the percentages of sulfur content, fixed carbon, oxygen and ash and other volatile content. The three types of coal provided were lignite, sub-bituminous, and bituminous which were located in Martin lake Texas, Montana, and Illinois respectively. Of the three coals the most promising coal for gasification seems to be the Montana sub-bituminous coal. According to Table 1, Martin Lake Texas Lignite is the cheapest of the three, however Montana sub-bituminous coal only costs \$1.70 more than Martin Lake Texas Lignite.

Of the three coals, Montana sub-bituminous has the lowest sulfur content, lowest moisture content, and highest fixed carbon content. With low sulfur content, there will be less acid gas to be removed during the acid gas removal process. Since it has the highest fixed carbon content it also will be able to produce the most synthesis gas.

Another factor taken into consideration was the sulfur content in the coal. The sub-bituminous coal was found to have the lowest percentage of sulfur content, 1.10% as compared to 1.30% and 3.74% of lignite and bituminous respectively. In high temperature processes all sulfur components in the feed are converted to  $H_2S$  or  $COS$ , which are undesirable components and require acid gas removal technology to be treated. Thus with less sulfur content it will be easier to remove sulfur based compounds. The oxygen content in the sub-bituminous is relatively high as compared to its counterparts, but it can be ignored since at such high temperatures, the oxygen is combusted completely before being converted to synthesis gas. Another advantage of using sub-bituminous coal is the low moisture content (10.50%) and the high fixed carbon content (59.82%). Unfortunately the Montana sub-bituminous coal has the highest ash content at 11.20%. This poses problems since during gasification, as certain

gasifiers, such as entrained-flow gasifiers must have ash flow continuously so that the slag-tap does not freeze up.

Therefore, taking into consideration the various properties and economic aspects of each of the given coals, it was concluded that the sub-bituminous coal from Montana is ideal coal for gasification.

#### *Choice of Gasifier Technology*

Three gasification technologies are available, namely moving-bed, fluid-bed, and entrained-flow gasifiers.

In the moving bed gasifier the coal slowly moves downwards and is gasified by counter current blast. It has the lowest oxygen demand. However, it operates at the lowest temperature, which inhibits the reaction rate and generally requires high maintenance costs. The fluid bed gasifier facilitates good mixing and does not require a membrane wall, thereby decreasing the overall cost. However, the conversion rate of carbon is lower as compared to the other two technologies due to some carbon lost with the ash. Also the temperature is limited by the softening point of ash, which results in a low purity syn gas due to the presence of pyrolysis products. Also, the fluid bed gasifier is appropriate for low rank coals like lignite, as opposed to sub-bituminous.

In the entrained flow gasifier, the fine coal particles react with concurrently flowing steam and oxygen. Since the gasifier operates at a high temperature, a good conversion of about 99% is obtained and the destruction of tar and oil yields a very pure syngas. However, the entrained flow gasifier has a high oxygen demand and the high ash content in the Sub-Bituminous would drive the oxygen consumption to higher levels. Overall, entrained flow gasifier was chosen as the gasifier technology for its high carbon conversion and purity of the resulting syngas.

A dry or a wet coal feed can be chosen for the entrained gasifier. A dry coal feed uses 20-25% less oxygen and has an extra degree of freedom that makes it possible to optimize the gas production. A wet coal feed requires more oxygen consumption and faces a loss in efficiency from the evaporation of water. However, the wet coal feed gasifiers are more elegant as compared to the complex and expensive ones used for dry coal feed. A dry coal feed was chosen for the entrained flow gasifier to reduce the required oxygen, which is the most expensive utility.



In dry-coal feed gasifiers, there are single stage and two stage gasifiers. In single-stage entrained-flow gasifier, high gas purity with only traces of hydrocarbons is obtained. It ensures low  $\text{CO}_2$  and high carbon conversion, in which almost all of the carbon is converted into CO. Hence, a non-selective acid gas removal can be employed, and the acid gas be routed directly to the Claus plant sulfur recovery. In a two-stage gasifier, there is an increase in the efficiency from 50% (single stage gasifier) to 50.9% (two stage gasifier). The consumption of oxygen is also decreased by 20%. The two-stage gasifier uses a refractory wall, which is cheaper than the membrane wall. However, the lower temperature of the second stage requires a longer residence time and a certain amount of tar leaves the syngas.

Out of the types of gasifiers mentioned above, the Noell gasifier and the CCP gasifier can be considered. The Noell gasifier is a single stage gasifier. One of the advantages of using a Noell gasifier is that the carbon particles from ash can be made to stay in longer in the reactor by as swirl in the top burner resulting in high carbon conversion. Another advantage is the use of simple rotational-symmetrical construction without penetration through the cylinder wall, which reduces equipment cost. However, the disadvantage of using the Noell gasifier is the fact that in conditions when a high ash coal is used, the gas yield is lower. The CCP gasifier is relatively new and is advantageous because it used air as the oxidant, which is readily available. The carbon conversion rate is 99.8%, with a variety of coals. Other advantages include lower  $\text{NO}_x$  and  $\text{SO}_x$  emissions, a reduction in solid waste generated, and the need for less cooling water. In addition to this, air-blown IGCC is better suited economically than the more expensive oxygen-blown IGCC. Reductions of 15% to 20% in  $\text{CO}_2$  emissions would also be beneficial and can cause much less of an environmental concern because of CCP system's feasibility in coupling with  $\text{CO}_2$  capture technology.<sup>1</sup> The two stage CCP gasifier technology was chosen due to its reduced oxygen consumption and use of a cheaper refractory wall.

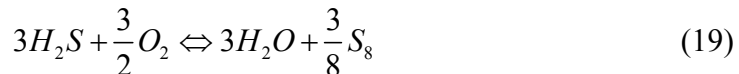
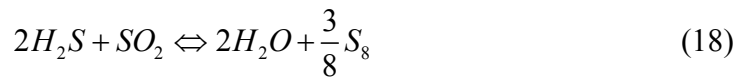
Overall, a two stage dry feed entrained flow gasifier (CCP technology) was chosen to maximize the carbon conversion and purity of the syngas and to minimize the costs of the most expensive utility (oxygen) and construction.

### *Choice of Acid Gas Removal Technology*

The Rectisol process is used in the acid gas removal process. It uses methanol as a solvent to separate acid gases such as hydrogen sulfide and carbon dioxide from feed gas streams. In the typical operating range of -30°C to -60°C, the Henry's law absorption coefficients of methanol are extremely high, and the process can achieve gas purities unmatched by other processes. Methanol, as a solvent, exhibits considerable selectivity, which allows substantial flexibility in the flowcharting of the Rectisol process. Both standard (nonselective) and selective variants of the process are regularly applied according to circumstances. The Rectisol technology is capable of removing not only conventional acid gas components but also, for example, HCN and hydrocarbons.

After the acid gas removal process, the acid gas produced is usually emitted in the form of H<sub>2</sub>S which tends to be highly toxic. It is necessary to convert this H<sub>2</sub>S gas into two alternative products of sulfur, either as liquid in the form of sulfuric acid, or solid elemental sulfur. If there is a local demand for phosphates, the market and production of sulfuric acid would be advantageous. If this is not the case, the elemental sulfur can be used for medicine, cosmetics, fertilizers and rubber products and is cheap to transport. For the production of elemental sulfur, the Claus process has become the most common and significant desulfurizing method. Since the invention of the process 100 years ago, Claus process has now been improvised into a two-stage process. It operates at a comparatively low temperature (200-300 °C) at the second stage to achieve much higher sulfur yields than had been possible with the original process.

The process is described as follows:<sup>2</sup>



In order to convert H<sub>2</sub>S to elemental sulfur during the Claus reaction, the catalysts with high activity under the highly reducing condition with the moisture should be developed.<sup>1</sup> The Claus technology can be divided into two process steps, thermal and catalytic. In the thermal step, hydrogen sulfide-laden gas reacts in a sub-stoichiometric

combustion at temperatures above 850 °C such that elemental sulfur precipitates in the downstream process gas cooler. Usually, 60 to 70% of the total amount of elemental sulfur produced in the process is obtained in the thermal process step.

To boost the sulfur yield, the Claus reaction is continued in the catalytic step with activated alumina or titanium dioxide. The catalytic recovery of sulfur consists of three sub steps: heating, catalytic reaction and cooling plus condensation. These three steps are normally repeated a maximum of three times. A cyclic process of the tail-gas treatment is also installed downstream of the Claus plant to incinerate or desorb the remaining sulfur, which is then recovered in a steam raising sulfur condenser.<sup>2</sup> Using two catalytic stages, the process will typically yield over 97% of the sulfur in the input stream. Over 2.6 tons of steam will be generated for each ton of sulfur yield.

#### *Choice of Water Gas Shift Reactors*

Different aspects of the water gas shift reactor must be considered when designing the reactor. The first thing to consider is the type of reactor. Either an adiabatic or isothermal reactor can be used. Adiabatic reactors have no heat transfer, but the temperature within the reactor increases due to the reaction being exothermic. Adiabatic reactor also requires cumbersome approximate or graphical methods.

Another consideration is the catalyst. According to the literature, the catalysts are manufactured by iron oxide with 5-15% Cr<sub>2</sub>O<sub>3</sub>.<sup>3</sup> The particle size, time in contact with the stream and the pressure - all affect the reaction rate. When comparing catalysts, the rate constant of 3/8 inch x 3/8 inch a catalyst particle was 10% less than that of 1/4 inch x 1/4 inch catalyst particle. This is mostly due to the fact that 60% of the surface area is available in the 3/8 inch x 3/8 inch tablet. The activity of the catalyst is largely dependent on the surface area. Also, at pressures of 450 lb/in gauge showed a decrease in the rate constant by 20-30%.<sup>3</sup> The optimal catalyst volume to achieve a given conversion is found to be with a T<sub>m</sub> (the temperature at which the reaction is maximized) is 100 °F less than the equilibrium temperature. Yet ranges from 50-100 °F were found to be acceptable.

## **Process Performance Summary**

### *Gasification Process*

The gasifier was modeled as a single RGibbs reactor. For the RGibbs reactor pressure was specified to be 32 bar according to the literature on dry feed, two stage, entrained flow gasifiers. The RGibbs reactor was also specified to calculate phase equilibrium and chemical equilibrium. 7500 tonnes of coal were inputted into the gasifier. The temperature of the outlet stream from the gasifier was 1453 K, which is in agreement with the literature on the temperature of the reactor. 1875 tonnes (metric tons) per day of water was inputted into the reactor at a temperature of 533.15 K and at a pressure of 101.35 kPa. 5625 tonnes per day of oxygen was added in at 1088.71 K and 3200 kPa. From the gasifier, 8566.44 tonnes of carbon monoxide and 400.26 tonnes of hydrogen were produced.

Adding more oxygen to the gasifier would increase carbon monoxide production but would also increase the temperature. Steam was added to the system to cool the process and to produce hydrogen gas. The syngas produced is a suitable amount but not the best we could possibly achieve since it was noticed from literature that more syngas can be produced with less coal. A lot of the coal used in the gasifier was also converted to carbon dioxide. It might have been more efficient if two RGibbs reactors were used to produce the syngas as well.

### *Solid Waste Removal (Ash and Gas)*

A splitter was used to remove the ash from the products stream. The remaining gases were then used in the acid gas removal process.

### *Acid Gas Removal*

Before the syngas was processed for acid gas removal it was cooled to 243.15 K using a heat exchanger in the simulation. The cooled syngas then entered into a Sep to separate out the hydrogen sulfide. In all, 3647.24 tonnes per day of hydrogen sulfide were removed. The acid free syngas then entered the water gas shift reactor.

### *Water Gas Shift Process*

The water gas shift reactor was modeled as a single RGibbs reactor. Reactor temperature was set isothermally at 350 K. The pressure was set at 32 bar. The reactor

was also specified to calculate the system with an equilibrium temperature approach of 10 °C.

Water was also added to the water gas shift to improve the conversion of carbon dioxide to hydrogen. The reactor produced 4740.80 tonnes of carbon monoxide and 675.59 tonnes of hydrogen gas. This is equivalent to 169.31 moles of carbon monoxide and 338 moles of hydrogen, resulting in a 2:1 ratio of hydrogen to carbon monoxide. The water gas shift was successful in producing the 2:1 ratio that we had hoped to achieve. Based on preliminary calculations the bare minimum composition of the syngas for methanol synthesis is 4380 tonnes per day of carbon monoxide and 650 tonnes per day of hydrogen. These numbers are based off of the assumption that the methanol synthesis reactors could achieve 100% conversion. Therefore having over the bare minimum was necessary since in reality 100% conversion is not realistic.

#### *Methanol Synthesis*

The methanol synthesis process was designed as 13 plug flow reactors connected in series. Splitters and coolers were placed in between the plug flow reactors. Splitters were used to separate the methanol after being synthesized in one reactor and before entering the next reactor. This was to prevent methanol buildup in the reactors and to avoid reverse reactions that would consume any synthesized methanol. The split streams were consolidated into a mixer before entering the refining process.

Coolers were used to ensure that the temperature of the syngas stayed close to chemical equilibrium but not at chemical equilibrium.

The 13 plug flow reactors used are not realistic but they were used for the purposes of producing 5000 tonnes per day of methanol in time to have the flow rates ready for distillation column calculations.

Before using the 13 plug flow reactor arrangement, parallel and recycle stream arrangements were considered and tested. For this system the parallel arrangement did not produce more methanol. Using recycle streams did not improve methanol production either. It is believed that if arranged properly both parallel and recycle stream arrangements can be used efficiently. However for this system it is believed that the

reason those arrangements are not effective are due to the kinetic information entered in the Aspen simulation.

The methanol synthesis process produces 5143.10 tonnes of methanol per day. Not all of the hydrogen and carbon monoxide gas converted completely to methanol. Thus it might be effective to add a recycle stream to further improve the conversion of carbon monoxide.

#### *Ethanol Simulation*

An RStoic reactor was used to simulate the parallel production of ethanol. The RStoic reactor produced 74.08 tonnes of ethanol per day. The stream that leaves the RStoic now contains methanol, ethanol, water and other gases. Since the distillation calculations only deal with methanol, ethanol and water, a separator was used to remove all the gases from the methanol stream so that the distillation calculations would be based purely off of methanol, ethanol and water.

#### *Methanol Refining*

The distillation column was modeled as a single RadFrac in the Aspen simulation. We had hoped to use one column so as to reduce costs but based on our results, a second distillation column may be required.

The stream entering the distillation column had a weight composition of 1.6% water, 96.92% methanol, 1.40% ethanol. The distillate from the distillation column had a weight composition of 1.34% water, 98.10% methanol, 0.56% ethanol. The AA methanol grade purity specifications require that the weight composition of the methanol be greater than 99.85% methanol on a dry basis, less than 0.1% water, and less than 50 ppmw ethanol. The distillate does not match these specifications.

To meet this amount it might be better to add in a second column and to add a second distillation column.

### **Project Economics Summary**

The total module cost is \$125,800,000 per year and total grassroots cost is \$155,800,000 per year. The following is a brief cost and profit economics summary of

the 1<sup>st</sup> and 5<sup>th</sup> year of operating the methanol synthesis plant. Five years was used as the basis for the economic and financial analysis.

The following is only a brief summary of the total economics analysis. A detailed analysis of the profit and loss, balance sheet, and cash flow statement can be found in the Appendix. Credit goes to Roland Esquivel, for the Excel spreadsheet used to calculate the financial statement values. In addition, the total capital cost and specific utility costs can be found in a table in the Appendix.

#### *1<sup>st</sup> Year Economics Summary*

Total Revenues are \$1,234,500. Maintenance is 3% of capital costs which is \$4,674,000.00. Total utilities costs are \$1,395,049,193.20. Total operating expenses comes out to be \$1,410,109,860 for the first year. Total profits are approximately -\$1,010,109,860.

#### *5<sup>th</sup> Year Economics Summary*

Total maintenance costs are \$5,234,800.00. Total utilities comes out to be \$1,859,418,437.00. Total operating expenses are \$1,876,286,383.00. Total profits for the 5<sup>th</sup> year are -\$1,390,524,848.00

#### *Internal Rate of Return*

Internal Rate of Return is calculated via the formula:

$$NPV = \sum_{t=0}^N \frac{C_t}{(1+r)^t} \quad (20)$$

where  $C_t$  is the annual cash flow, NPV is the net present value and  $r$  is the internal rate of return. For this calculation, the values of cash flows were calculated and NPV was set to 0. Using solver on Excel, the IRR or  $r$  value could be found.

However, since operating expenses are larger than revenues such that the calculation for IRR will never converge. The IRR cannot be found and the plant will never be profitable.

#### *Economics Conclusion*

It is not likely that this plant will make a profit in the long run. We consider the plant to not be economically feasible especially after 5 years the losses continue to mount

further into the billion dollar range. Internal rate of return was not found because no solution exists to the problem.

### **Process Description**

Coal gasification involves the conversion of coal into carbon monoxide and hydrogen (also known as synthesis gas) in the presence of oxygen. First, the coal is prepared in the pre-processing stage, which includes crushing, sizing, and drying. It is then sent to a gasifier, where it reacts with oxygen ( $O_2$ ) to produce carbon monoxide (CO) and hydrogen ( $H_2$ ) gas, which is collectively known as syngas. The gasification process is followed by acid gas ( $H_2S$ ,  $CO_2$ ) removal from the syn gas. The removal of these impurities is essential in order to maintain a high purity of the methanol product. The selected method needs to remove sulfur to a level of 0.1 ppmv or lower while maintaining a high selectivity for  $H_2S$  relative to  $CO_2$ . The product gas is then sent through a water-gas shift reactor in order to change the syngas ratio ( $H_2$ : CO) to the optimal ratio (2:1) for methanol synthesis. The water-gas shift reaction is a temperature dependent equilibrium reaction. The resulting gas goes into a methanol synthesis reactor to produce methanol and small quantities of ethanol. Finally, the methanol is refined to produce the AA methanol grade purity, 99.85% w/w methanol (dry basis), less than 0.1% w/w water, and less than 50 ppmw ethanol.

### **Major Equipment With Sizing**

All the major equipment and specifications are listed as follows:

**Table 1: Major Equipment With Sizing**

<b>Equipment</b>	<b>Height(meters)</b>	<b>Diameter(meters)</b>
Gasifier	31.79	15.90
Acid Gas Removal	21.20	10.50
Water Gas Shift Reactor	23.8	12.00
Methanol Synthesis Reactor (13x)	6.09	2.89
Methanol Distillation Column	69.75	4.91

### **Environment & Safety Considerations**

Different stages of the coal to methanol process have different environmental and safety considerations. Coal gasification process operates at high temperatures and



pressures conditions and also employs the use of combustible materials, which can be hazardous. In order to control and prevent fire and explosion risks, measures, such as providing early release detection that utilizes smoke detector and pressure monitoring of gas and liquid conveyance system, are recommended. The gasification process may also generate pollutants such as hydrogen sulfide ( $\text{H}_2\text{S}$ ), carbonyl sulfide ( $\text{COS}$ ), carbon monoxide ( $\text{CO}$ ), ammonia ( $\text{NH}_3$ ), and hydrogen cyanide ( $\text{HCN}$ ). These gasses can be treated by the installation of a sulfur recovery process to avoid emissions of  $\text{H}_2\text{S}$  (e.g., clauss process) as well as the installation of scrubbing processes and incineration devices. Use of oxygen requires special attention and an important aspect is material selection and system geometry. Materials are selected to keep the ignitability of the material and its capability of sustaining a fire in an oxygen atmosphere to a minimum. Velocities in oxygen lines are generally kept low as a measure to limit the energy release on impact of any particles in the system. An additional measure to limit the ignition risk is to avoid sharp bends in piping where turbulence can increase local velocities much above these limits. Oxygen compressors enclosed by a fireproof wall are used to ensure any personnel is not put at risk [8]. During shutdown, the gasifier is often nitrogen blanketed to avoid corrosion. Repairs are carried out inside the gasifier, and no other gases other than air are present. Drawing a good vacuum and breaking it with air is the best way to ensure the above. This operation can be repeated several times to ensure all noxious gases are removed.

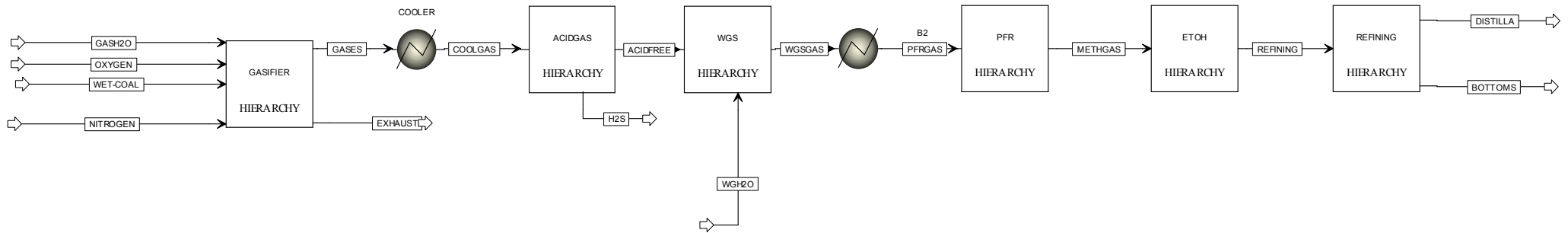
In the water gas shift reactor, the high temperature proves to be a hazard. The toxic gases in the water gas shift and the Acid gas removal are also sources of the hazard. The  $\text{H}_2\text{S}$  produced in the process is corrosive and can make steel brittle. The environment gets contaminated with the various greenhouse gasses ( $\text{CO}_2$ ,  $\text{CO}$ , and  $\text{CH}_4$ ) that are present in the process. The release of  $\text{SO}_2$  poses an environmental hazard as it is the major cause of acid rain. Being highly toxic, it also poses as a health concern. To prevent these compounds from being emitted into the atmosphere, all operations need to be well contained. Relief valves and sprinklers need to be used when designing and building the process.

During methanol synthesis, most of the syngas produced during the coal gasification process is used for production of methanol. Methanol is toxic if ingested,

inhaled, or absorbed through the skin. While carefully handling the methanol, it would be recommended to wear skin protection. Methanol synthesis requires the use of catalysts and their handling should be given special attention. Unloading spent catalyst, which may not have been adequately oxidized in situ, can potentially be a source for spontaneous combustion.

## **References**

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**Figure 1: Aspen Flow Diagram**

	GASH2O	OXYGEN	WET-COAL	NITROGEN	GASES	EXHAUST	COOLGAS	ACIDFREE	H2S	ACIDFREE	WGH2O	WGSGAS	PFRGAS	REFINING	DISTILLA	BOTTOMS
Substream: MIXED																
Mass Flow kg/hr																
H2O	78125	0	0	0	80754	5	80754	80754	0	80754	21875	107	107	3726	2810	916
N2	0	0	0	4531	4191	4531	4191	4191	0	4191	0	4191	4191	4191	0	0
O2	0	234376	0	5	0	5	0	0	0	0	0	0	0	0	0	0
NO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2	0	0	0	0	16678	0	16678	16678	0	16678	0	28150	28150	375	0	0
CL2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HCL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	0	0	0	0	356935	0	356935	356935	0	356935	0	197533	197533	10198	0	0
CO2	0	0	0	0	127351	0	127351	127351	0	127351	0	377802	377802	371910	0	0
H2S	0	0	0	0	3647	0	3647	0	3647	0	0	0	0	0	0	0
CH4	0	0	0	0	254	0	254	254	0	254	0	254	254	254	0	0
CH3OH	0	0	0	0	0	0	0	0	0	0	0	0	0	214296	205782	8514
C2H5OH	0	0	0	0	0	0	0	0	0	0	0	0	0	3087	1165	1922
Total Flow kmol/hr	4337	7325	0	162	28665	162	28665	28558	107	28558	1214	29772	29772	16128	6603	358
Total Flow kg/hr	78125	234376	0	4536	589809	4541	589809	586162	3647	586162	21875	608037	608037	608037	209757	11352
Total Flow l/min	3151032	347657	0	2871	1813485	2146	247015	255512	63	255512	23441	447144	254499	338635	5896	310
Temperature K	533	1089		405	1453	307	243	251	251	251	510	350	515	515	384	386
Pressure atm	1	32	32	32	32	32	32	32	32	32	32	32	84	32	5	5