



IPRO 346 – Fall 2006
Design of Coal Desulfurization Processes to Improve the
Environment
Final Report

Introduction

The goal of IPRO 346 is to determine a means for the desulfurization of coal prior to combustion for application in large-scale steel production. The fuel coke is a vital component of industrial steel production processes. Coke is produced by baking coal in a blast furnace and later used to produce steel.

The presence of sulfur in coal effects purity and quality levels of the output products, specifically coke and steel. Pre-combustion desulfurization of the coal would lead to a higher quality coke consequently resulting in higher quality steel being manufactured. Additionally desulfurized coal has added utility since if combusted for traditional uses such as power or heat generation it will only release a acceptable modicum of Sulfur Dioxide into the atmosphere. It is for this purpose that IPRO 346 has been organized, with an objective of researching and developing a method for coal desulfurization that is both industrially and financially viable.

Background

What is coal?

Coal is a carbonaceous compound unique for its large yield of energy, for which it is used as a major industrial and power generating resource. Coal formation begins when plants die and undergo incomplete decomposition due to an anaerobic environment, such as the bottom level of a swamp. Over time, the swamp drains and new layers of land form on top of the plant matter. The pressure caused by the new layers forces almost all of the moisture out of the decomposing plants, leaving mainly the organic matter to rest. This then fossilizes into coal.

Coal is composed of four general resources: Carbon (75-84%), Oxygen (5-13.5%), Hydrogen (5-6%), and Sulfur (0.7-5%). In addition, coal contains a variety of trace elements, such as arsenic, boron, beryllium, cadmium, chlorine, cobalt, chromium, copper, fluorine, mercury, lithium, manganese, molybdenum, nickel, phosphorus, lead, sulfur, tin, selenium, thorium, uranium, vanadium, and zinc, (Source: "Coal Geology of Illinois", ISGS). Illinois coals unlike other coals within the United States are generally known for their higher calorific value and high sulfur content. The two main Illinois seams, the Springfield seam and the Herrin seam, have between one and four percent sulfur and calorific values between 9,700 -12,700 BTU (British Thermal Units)/lb. These coals will be discussed more extensively however later in the report.

Most of Illinois rests on a very wide bed of coal known as the Illinois basin, which also extends under parts of Indiana, and eastern Kentucky. The only areas of Illinois not underlain by coal are in the northern fourth of the state and narrow strips beside major waterways. The beds of coal with the lowest sulfur content in Illinois are all in the southern and central portions of the state, causing a general focus of mining to be concentrated within that area.

Coal's high burning potential makes it the ideal source fuel for a large percentage of power plants within the world. Another advantage of coal is that the resource is widely available, and when dealing with power generation, it does not depend on specific weather conditions like its counterparts in solar or wind power. Coal can also be easily stored after mining. Lastly, coal is also portable, allowing power plants to be built in areas where alternative forms of power generation, such as hydroelectric dams, may not be feasible.

However, when coal is burned the sulfur it contains is released into the air as sulfur dioxide as well as other emissions, which increases haziness, irritates the lungs, and is a major component of acid rain. Efforts by watchdog groups such as the EPA to reduce pollution have led to an increased interest in methods to remove sulfur compounds from coal emissions. Emission factors of coal will be examined in greater detail later in the report.

Types of coal

Coal is classified into four major types or ranks that are based on the age and depth of each coal member to differentiate between types with varying carbon content and energy yields. The four ranks are Lignite, Sub-bituminous, Bituminous, and Anthracite.

Lignite - often referred to as "brown coal" - is the softest of the four types. It ranks the lowest in carbon content and is the youngest form of all coals. The moisture content of lignite coal is the highest mainly due to its young age. According to the American Coal Foundation, the majority of lignite coal is mined in Texas, but large deposits are also found in Montana, North Dakota, and some Gulf Coast states. It is primarily used for steam-electric power generation, while the heating content of this coal ranges between 4,000 and 8,000 BTUs-per-pound (British thermal units per pound) with a carbon content of 25%-35%.

Sub-bituminous is a medium soft coal which contains lower moisture content than its counterpart lignite coal. Sub-bituminous is mined mainly in a half-dozen Western states and Alaska. Like lignite, it is mainly used as fuel for steam-electric power generation. The heating content of this coal lies between 8,000 and 13,000 BTUs-per-pound while its carbon content is 35%-45%. According to American Coal Foundation, sub-bituminous has lower sulfur content than other types, which makes it attractive for major power generation because it is clean burning potential.

Bituminous coal is one of the two "hard coals". The moisture content in Bituminous coal is again very low due to its increased age. This coal is the most abundant form in the United States and it is mined primarily in the Eastern and Midwestern region of the US. It is used primarily for power generation and manufacturing coke for the steel industry. The heating content of bituminous is between 10,500 and 15,500 BTUs-per-pound with a relative carbon content of 45%-85%.

Anthracite is the highest rank and the hardest of the all types of coal. It is mined mostly in the eastern Pennsylvania region. It is used for residential and commercial space heating, municipal water purification, and treatment plants. The heating content of anthracite coal tends to be over 15,000 BTUs-per-pound mainly since its carbon content ranges between 85%-95%; however, it is noted by the American Coal Foundation that anthracite is not a very prevalent coal within the U.S. coal market.

In the state of Illinois, Bituminous coal is the only class of coal present. As stated earlier, Bituminous coal is generally used for power generation and within the steel industry for the generation of coke. However, within the coal in Illinois lie seven distinct subgroups of coal. Each of these groups is named for the various locations in which they were found within the state, and also by the select depth

of the coal field under the surface of the earth. The six major groups are as follows: Rock Island (#1), Colchester (#2), Sumnum (#4), Springfield (#5), Herrin (#6), and Danville (#7). Out of these select groups, the most predominantly used types are the Springfield and Herrin coal seams. Both are known for a relatively high energy output and a rather low sulfur percentage within the coal structure.

Springfield coal, mainly found in mid-central and southern Illinois, is Illinois' highest energy coal. The coal, which is usually surfaced mined, yields a calorific value of 12.4-12.7k BTU/lb when at its peak. However, since the burning potential is higher than other coals in the region, Springfield coal also has a moderate sulfur percentage which lies between 3-4% of the coal. The ash percentage also tracks in at 3-4%, which factors in during the burning process of this particular type.

Herrin coal, known for its generally low sulfur content, is Illinois's highest mined coal and is located in the southern areas of the state. The advantage of using this coal for power production lies within the general sulfur content of the coal, which ranges from .5-2.5%. Although this coal does not produce as much energy as Springfield coal, approximately 10.4-11.1k BTU/lb, it is more widely incorporated into power generation. The ash content of this coal however, is very high, ranging from 8-12%.

Coal Sources

There are two types of coal mines; surface and underground. Surface mining is a relatively cheap process, but yields less energy coal than the underground counterparts, mainly since the coal has a younger age. However, due to the increasing risk of underground mining, the surface mining industry within Illinois has flourished greatly.

Coal Emissions and Harmful Compounds

The utility of coal is partly offset by the environmental damage that its use creates. Its combustion releases harmful products, the most prevalent of which are sulfur dioxide, sulfur oxide, and nitrous oxide.

Sulfur dioxide is a gas that is one of the main contributors to the depletion of the ozone layer. After the combustion of coal, the majority of sulfur within the fuel is converted to this gas which exits with all the excess coal fume gases. The most effective way to lower the amount of sulfur dioxide in the emissions is to either utilize a scrubbing of the gases upon exit, or rather to deplete the sulfur from the coal before combustion by a use of scrubbing or other various methods created. The EPA regulates the emissions on coal at 2.5 pounds of SO₂/mmBtu (million British thermal units), which is stagnantly based on heat input. Pre-combustion desulfurization is the most effective means of reducing the sulfur dioxide output.

Another sulfur compound that formed in coal is sulfur oxide. This form is generally present in the coal bed prior to mining. Sulfur oxide can be best eliminated by the injection of lime or dolomite into the coal bed. This process will then remove the sulfur oxide at a relatively fast rate, and can also be used during the combustion stage of the coal use.

Nitrous oxide is not part of the coal or formed directly through combustion, but rather is produced when the coal is scrubbed in order to eliminate the select sulfur compounds through the formation and oxidation of hydrogen cyanide. It has been found that by using a triple combustion chamber technique to burn the coal has greatly reduced this emission, since it has not been able to form under these conditions.

Overall it is evident that the use of Springfield and Herrin coal are very beneficial to the Illinois power industry and abroad. However, it is crucial that the implementation of desulphurization coal be used in order to lower its potential to harm the environment.

Coal Selection for this Project

In order to realistically model the process being researched by I-Pro 346, one of these types of coal needed to be chosen. The group's decision was to use Illinois #6, or Herrin coal, which has relatively low sulfur content and also has an even distribution of both pyritic and organic sulfur. The following tables display the amounts of various compounds found in Illinois #6 coal.

Table 1: Composition of Illinois #6 Coal

Sample Number	Ultimate Analysis1				
	Hydrogen %	Carbon %	Nitrogen %	Oxygen %	Sulfur %
Illinois #6	5.07	66.15	1.40	12.46	3.40
Illinois #6	5.01	64.80	1.28	12.85	4.21
Average	5.04	65.475	1.34	12.655	3.805

¹ National Coal Resources Data System, "US Coal Quality Database" <http://energy.er.usgs.gov/products/databases/coalqual/index.htm>

Table 2: Heat of Combustion and Sulfur Amounts of Illinois #6 Coal

Sample Number	Heat of Combustion ¹		Forms of Sulfur ¹		
	Kcal/kg	Btu/lb	Sulfate %	Pyritic %	Organic %
Illinois #6	6588.96	1872	0.08	1.34	1.98
Illinois #6	6473.52	1664	0.27	2.31	1.63
Average	6531.24	1768	0.175	1.825	1.805

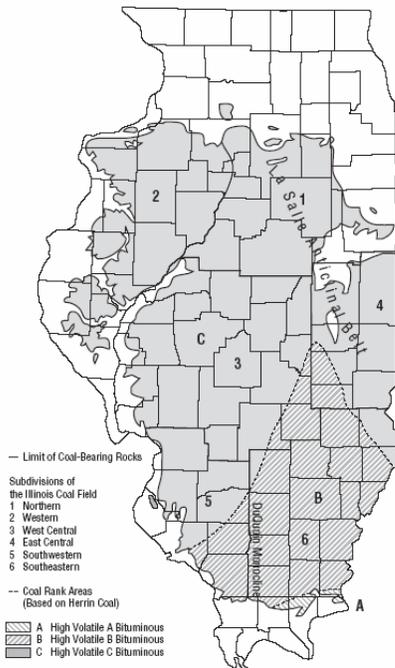


Figure 1: Subdivisions of the Illinois Coalfield. Areas of high volatile A, B, C bituminous rank coals.²

Illinois #6 coal is mined extensively in the state and accounts for 40% of the total coal mined. This type of coal is found to be in the best quality and most abundant in the Jefferson-Franklin-Williamson counties. This area is known as the "Quality Circle", covering 250 square miles. The sulfur content is an average of 1.5% in this area.

² Russell Jacobson, "Coal Geology of Illinois" 2003

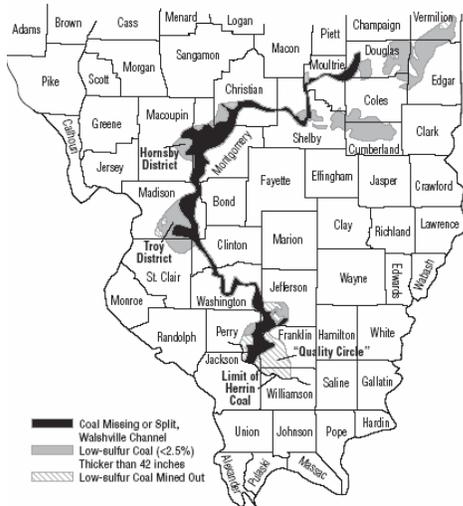


Figure 2: Location of IL#6 Coal

What is coke?

When coal is heated to temperatures up to 1100°C in an anaerobic environment, it is stripped of many of its components including tar, ammonia, water, light oils, a gas known as coke oven gas (which is in return reused to heat the furnace), and sulfur compounds. This process is known as carbonization. The leftover substance, referred to as coke, is composed of many crystallographic forms of coal along with ash-like remains containing many of the minerals that survived the carbonization. Also present after carbonization are bits of sulfur that were not completely removed during combustion with the rest of the sulfuric compounds. The following is a table listing the amounts of the different components found in coke, adapted from a table found on the American Iron and Steel Institute’s website:

Physical Components of Coke	Composition % by Weight
Ash	8.0 - 9.0 %
Moisture	2.5 – 5.0 %
Sulfur	0.65 – 0.82 %
Volatile Matter	0.5 – 1.5 %
Alkali (K ₂ O+ Na ₂ O)	0.25 – 0.40 %
Phosphorus	0.02 – 0.33%

Table 3: Coal Composition

History of Coke

The production of coke was first devised by Sir Henry Platt in 1603. England at the time was having problems producing iron because they relied heavily on using wood, which was becoming both limited and expensive. Knowing that burning coal gave off unwanted smoky fumes, Platt suggested that coke be charred in a way similar to how charcoal is made from wood. It took 39 years for the process to actually be used, as it was in Derbyshire to roast malt to prepare it for brewing beer. In 1709 a former apprentice from a malt mill named Abraham Darby produced coke in a blast furnace and used it to produce cast iron; however, this technique remained expensive until the introduction of steam power. The resulting fall in the price of iron production helped lead Europe into the Industrial Revolution.

Coking Mechanism

The importance of pre-combustion coal desulfurization can be best realized by studying the mechanism used to produce coke for blast furnaces. Coal is baked in a sealed, airtight oven at temperatures that go up to 1473 K in a process that purifies the carbon by removing water, radicals and other volatile components to fuse the pure coal particles together. The preliminary requirements for the coking process to be undertaken are a constant heat supply that is normally provided by gas burning flues within the oven and contact between the coal particles throughout the carbonization process. The latter is achieved by filling the coal oven vertically through the dropping of pulverized coal particles from a height.

As the coal is heated, radicals and light volatile molecules that have lower molecular weights than coal are liquefied or turned to gas products. While most of the gases escape, the surface tension of the liquids causes the coal particles to adhere to each other and aids in the fusing process that follows. With the heat source on the oven walls, the layers of coal closest to the walls are the first to completely stabilize by loss of volatile components and start to soften. The partially fused coal gains plastic-like properties and binds to form an envelope that moves inwards as the coking process continues. Coal closer to the centre of the oven is then heated and volatile particles are driven off in gases as the carbon crystal structure purifies. The coking process is completed once all volatiles have been removed from the coal, and the envelope of plastic-like coal has converged at the centre of the oven, leaving behind pure coke.

The mechanism is a time consuming one; taking 18 hours or more at temperatures of 1200°C. This inefficiency can be exacerbated by large amounts of impurities in the coal; in particular sulfur, the removal of which requires added time and heat in order to purify the coke produced. Efficient desulfurization of the coal before coking allows the coking process to proceed at faster rates with lower energy expenditure.

Forms of Sulfur in Coal

Sulfur in coal can be classified into two main types; organic and inorganic. These types can be further subdivided. Inorganic forms of sulfur include: Pyritic Sulfur having the general formula FeS_2 , which takes on two crystalline forms Pyrite (cubic) and Marcasite (orthorhombic); and Sulfate Sulfur, or gypsum, which is formed through the oxidation of Pyritic forms and is generally of the formula $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$. Organic forms of sulfur are actual bonded to the structure of the coal and can be found in the form of: Mercaptans or Thiols (RSH); Sulfides or Thio-ethers (RSR'); Disulfides (RSSR'); or Aromatic Systems containing a thiopene ring (Wheelock).

Purpose

The purpose of this IPRO was to find and model a method of desulfurizing coal for the generation of coke in an industrially and environmentally sound manner. The environmental concerns and industrial concerns can both be accounted for in one simple number – the percentage of total sulfur removed from the coal that is being treated. Consequently optimizing our SO₂ and H₂SO₄ generation reactions in our fluidized bed was the paramount concern of this IPRO.

Research Methodology

Rather than forming two or three main subgroups for this project, IPRO 346's method for project efficiency involved implementing a variety of subgroups based on select topics over the course of the semester. These groups researched for a week or two and worked towards certain deadlines. After the task was completed, the group members moved towards the next task to continue stepping toward completing the overall IPRO objective.

Groups were broken up into different subgroups, listed in the Assignments section. Research was performed giving the group a solid background on coal and coke, (as listed in the Background section) and various desulfurization methods. A summary of the different methods ensues.

1. Biological Methods

Microbial desulfurization of coal, or the use of sulfur-eating bacteria to extract sulfur from coal products, has been a field that has shown great growth within the past years. By using select bacterium, mainly thermophilic bacterium known for their susceptibility to survive at extreme temperatures, coal could be selected degraded of both organic and inorganic sulfur compounds which exist within the fossil fuel.

Although many organisms exist, each of these organisms are extremely selective on which sulfur is used as their primary food source. *Thiobacillus ferrooxidans* and *Sulfolobus acidocaldarius* are used for the removal of inorganic pyritic sulfur within coal, while *Sulfolobus brierleyi* and *Sulfolobus solfataricus* focus primarily on the removal of organic sulfur.

When desulfurization procedures are undertaken, great care on the conditions in which these organisms are kept, must be established. Bacteria in general, are very selective in the surrounding environment. Thermophiles require a high temperature, approximately 45-70 degrees Celsius, a highly acidic pH, and a relatively low salt concentration in order to retain function.³ Also, in order for an effective amount of coal to be desulfurized, the coal members must be subjected to the bacteria in rather small particles to ensure that the organism can

³ Jorjani, E., Rezai, B., Vossoughi, M., Osanloo, M. "Biodesulfurization of the Tabas Deposit Coal by Microorganisms." *Journal of Mining Science* 40.3 (2004): 310-319.

extract the maximum sulfur output. Fluctuations in the conditions above can lower the efficiency of the desulfurization process, and possibly kill off the bacterium if the conditions are too harsh.

One of the more known bio-desulfurization procedures for coal was committed using the bacterium *Sulfolobus acidocaldarius*. Within the experiment, coal was ground into a slurry mixture and subjected to this bacterium for a series of days. Within the slurry mixture, yeast and glucose members were present to help stabilize the exponential growth of the bacterium above. After ten days of exposure at optimal conditions for the bacterium, the coal was removed via bacterial filtration from the solution and the sulfur concentration was determined by using HCl to extract sulfate particles from the remaining coal. The results showed that 96% of the inorganic sulfur present within the coal was removed, yielding 50% total sulfur removal⁴.

Pre-combustion bio-desulfurization has notable advantages over physical and chemical methods. First, lower capital is needed for startup on the procedure and operating costs are generally kept at a low. Second, lower energy loss is portrayed within the coal, because specific elements of combustion are not extracted from coal particles as shown in the other processes. Third, it is less energy intensive than chemical processes because it operates at lower temperatures and pressures than competing chemical counterparts⁵. Lastly, the inorganic sulfur removal rates of these organisms are very high, although a problem can be established from the lower yield of total sulfur degradation. In conclusion, bio-desulfurization processes of coal are very useful when dealing with the inorganic products of the sulfur compounds present in the system, but extended time and low sulfur yield make this area undesirable. Hopefully, within the future, more emphasis will be set on this field to improve the process and provide a cheap and effective way to remove all types of sulfur from coal.

Microbial Desulfurization of Coal

There are several types of microorganisms that are used in the coal desulfurization process. *Thiobacillus ferrooxidans*, *Thiobacillus thiooxidans*, and *Thiobacillus acidophilus* are major organisms used for the removal of pyritic sulfur from coal⁶. *Sulfolobus acidocaldarius* is used for the removal of organic sulfur as well as portions of inorganic pyrite from coal. In addition, *Sulfolobus brierleyi* & *Sulfolobus solfataricus* are also used for the removal of organic sulfur; the latter one has higher rates and higher percentages removal of organic sulfur in the coal desulfurization process¹⁹.

Effective biodesulfurization of coal depends upon several conditions for success. These are comprised in specific pH, coal particle size, pulp density,

⁴ Kargi, F., Robinson J., "Removal of Sulfur Compounds from Coal by the Thermophilic Organism *Sulfolobus acidocaldarius*" Applied and Environmental Microbiology Oct. (1982): 878-883.

⁵ Durusoy, T., Ozbas, T., Tanyolac, T., Yurum, T. "Biodesulfurization of Some Turkish Lignites by *Sulfolobus solfataricus*." Energy & Fuels 6 (1992): 804-808.

⁶ Durusoy, T., Ozbas, T., Tanyolac, T., Yurum, T. "Biodesulfurization of Some Turkish Lignites by *Sulfolobus solfataricus*." Energy & Fuels 6 (1992): 804-808.

temperature, and reactor mixing rate⁷. The desulfurization of coal is known to decrease as pH shifts acidic to basic conditions. Coal particles of smaller diameter are more effective for removal of sulfur by biodesulfurization process due to increased surface area ratio. In addition, the effective sulfur removal in coal decreased as pulp density and temperature increased.

Overall, there are several advantages and disadvantages of using microorganisms for successful coal desulfurization. Precombustion biodesulfurization has notable advantages over physical and chemical methods, by encompassing lower capital and operating costs¹⁹, while giving lower energy loss and coal refuse¹⁹. Also, the process is less energy intensive than chemical processes since it operates at low temperature (25-75 °C) and low pressure¹⁹. These factors lead to reductions of 50-60% and select organic sulfur reductions of 80-90%^{19,20}. However, disadvantages of these methods lie in low removal percentages during large scale implementation, yielding removal rates of too low standard to make this process economically attractive to industry¹⁹.

2. Chemical Methods

IGT Hydrodesulfurization

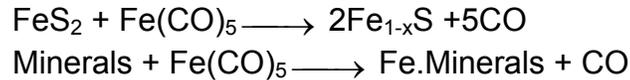
IGT hydrodesulfurization is a two step process for coal desulfurization that uses a combination of both oxydesulfurization and hydrogenation treatments. This technology was developed by The Institute of Gas Technology (IGT). To start, pulverized coal is placed in contact with air in a fluidized bed reactor. After this first reaction, coal is subjected to hydrogen in a second fluidized bed reactor. Reactor conditions lie at 400⁰C for first reactor, and 800⁰C for second reactor⁸, while both operate around atmospheric pressure. For bituminous coal, this process desulfurizes approximately 25-30% of total sulfur within the first fluidized bed reactor. The second fluidized bed reactor removes sulfur present in the form H₂S. The overall efficiency of the *IGT* process is 83% of total BTU if all products are recovered (including steam). The major disadvantage of this process, however, is that oxidation of the coal destroys the ability of the coal product to be manufactured into coke.

Magnex Process

The Magnex process uses chemical reaction to convert slightly magnetic pyrite and nonmagnetic minerals into a paramagnetic substance. This method uses two reactions to decompose and reacts the pyrite with other minerals. The removal of sulfur is committed by a low intensity magnet.

⁷ Jorjani, E., Rezai, B., Vossoughi, M., Osanloo, M. "Biodesulfurization of the Tabas Deposit Coal by Microorganisms." *Journal of Mining Science* 40.3 (2004): 310-319.

⁸ S. Komar Kawatra, Timothy C. Eisele, "Coal Desulfurization, High-Efficiency Preparation Methods". Page 332.



A magnetic relationship is created when metallic iron converts the surface of the pyrite particles into pyrrhotite. For the process to operate, coal has to be heated and grinded to less than 1.41mm and held at 170C, making a grinder, low temperature heater, batch reactor, and magnetic separator crucial to this process. The technology involved in this method is very simple, allowing the removal of volatile compounds, elemental sulfur, and pyritic sulfur. This technology has been implemented on the pilot plant scale with bituminous coal. The *Magnex* process has recorded to remove 92% of pyritic sulfur, while having BTU recoveries ranging from 86% to 96%.²²

Chemical Comminution

Chemical comminution provides a simple route of crushing coal for mineral liberation of sulfur elements. First, coal is treated with ammonia solution resulting in selective breakage. As the coal particle size decreases, the amount of mineral matter liberated rises. However, extended crushing of the coal particles leads to high equipment costs. Using this process pyritic sulfur can be removed without grinding to extremely minute sizes. After cleaning the product, the resulting material contains 80-90% less pyritic sulfur and 50-60% less ash than the original sample.

Laboratory Extraction

When looking into laboratory sulfur extraction methods, the only feasible desulfurization results have occurred on a small scale. Within these methods, the removal rates of pyritic and organic sulfur were high, but implementation of these processes on a larger scale would lead to financial ineffectiveness due to the high reagent costs involved along with the added cost of removing chemical residues created as chemical byproducts.

Methods of using potassium permanganate, sodium hypochlorite, or other chlorinated solvents as oxidizing agents were also considered. However, the use of sodium hypochlorite is ineffective in the removal of pyritic sulfur and leaves behind chlorine deposits of 2-2.7% within the coal, therefore requiring additional cleaning of the subjected coal prior to combustion. Potassium permanganate is more effective for sulfur removal, but purchase costs outweigh total effectiveness, since the usage of additional chemicals, such as 1,1,1-trichloroethane as a pre-cleaning fluid and HCl for a post-filtration wash, make it an extremely expensive procedure when committed on a large scale.

Supercritical fluid extraction and the Hydride reduction method with SET (Single electron transfer method) and BASE (Lochmann's base reactive mixture) were also considered as feasible processes, but the constant upkeep of high

pressures and specific heat levels needed for the supercritical extraction would make the process an inconvenient procedure for application to several hundred tons of coal each day. The Hydride reduction with SET and BASE, although less expensive, is more time consuming since the combination of the three methods ultimately reducing sulfur levels to below 1% require over 54 hours for complete desulfurization. As all these processes involve high costs for large quantities of these chemical reagents, as specific processes also require additional pressure and temperature controls, the consensus was made that the chemical laboratory desulfurization processes would be unviable for application of coal desulfurization on a medium to large scale.

Potassium permanganate

Desulfurization by potassium permanganate requires preliminary cleaning of the coal by heavy media separation using 1,1,1-trichloroethane, prior to desulfurization. The coal is then ground and subjected to a cycle of oxidation with 6% potassium permanganate solution, which is followed by a filtration cycle, and washed in hydrochloric acid and later, hot water. The procedure is repeated three times, with total sulfur reduction of 63%. The process is most effective in the removal of pyritic sulfur, by successfully extracting 97%⁹.

Sodium hypochlorite

Sodium hypochlorite is among the least effective chemical desulfurization methods due to the low degree of pyritic sulfur reduction. This process treats coal with a sodium hypochlorite solution, and then washes the solution in a sodium carbonate solution. This procedure is repeated twice ultimately reducing overall sulfur by 49.5%. However, the use of sodium hypochlorite for sulfur extraction causes residual chlorine to be left within the coal, (around 2-2.7%), which requires pre-combustion cleaning requirement prior to application¹⁰.

Supercritical fluid extraction

Within supercritical fluid extraction, carbon dioxide is used under supercritical conditions of 54.72 MPa and 755K to remove sulfur from coal in a chromatographic column. This is one of the most effective chemical desulfurization methods, having the ability to remove other volatile materials within the coal as well as sulfur members, but the high pressure and temperature conditions lead to highly prohibitive costs when this process is applied to anything larger than laboratory scale. In addition, proper disposal of the solvent byproducts increase maintenance costs further¹¹.

Peroxyacetic Acid

⁹ <http://www.osti.gov/bridge/servlets/purl/10188072-wUqAeu/10188072.PDF>

¹⁰ http://pubs.acs.org/cgi-bin/abstract.cgi/enfuem/1989/3/i04/f-pdf/f_ef00016a009.pdf?sessid=600613

¹¹ http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=PubMed&list_uids=9487670&dopt=Abstract

Peroxyacetic Acid is two-stage process consisting of coal dispersal in glacial acetic acid (CH_3COOH) between the temperatures of 21-104C. Coal is then mixed with 30% hydrogen peroxide (H_2O_2), and filtrated, while reacting in sodium bicarbonate mixed with methanol at 350-450C. If this method is used in conjunction with a base in an inorganic solvent, peroxyacetic acid desulfurization removes 85-95% of total inorganic sulfur.¹²

Oxidative Treatments

Oxidative treatment offer a promising number of chemical methods to successfully desulfurized coal. These methods focus on the removal of both pyritic and organic sulfur via attachment to sulfur by means of electronegative particles.

Metallic Salts

The Meyers process and select methods involving Ferric Chloride, lay the path for successful desulfurization, since they integrate well with certain physical desulfurization methods (magnetic and froth flotation) and operate at atmospheric pressure. However, the reactants used in this process are very expensive, which include NaOH in conjunction with a group I or group II metallic salt. Considering a coal to treating solution (.5M ~ 1M) ratio of 1 / 5 to 1 / 20 (Grant, Coal Desulfurization, US Patent #4167397) this process was seen as not economically viable in comparison to alternative procedures. To further support this conclusion, this method only removes approximately 20% of total sulfur content within Illinois #6 coal, which lies far below the yield for this project.

Chlorinolysis

Chlorinolysis was another method found to be prohibitively expensive due to reactant and operating costs. In addition to expensive reagents, this method also requires high temperature conditions. Additionally, the resulting coal must be dechlorinated via Nitrogen or Hydrogen gas, which result in excess NOx emissions (another controlled emission). This method does however result in high sulfur removal yielding 81% total sulfur removal (Ravindram et al, Fluidized Bed Desulfurization, US Patent # 4511362).

Oxydesulfurization

When comparing to other chemical methods, Oxydesulfurization provides high sulfur removal with the benefit of low reagent cost. Besides coal, only water and air are needed to complete this process. This method operates under high temperature and pressure measurements in order to fix atmospheric oxygen to

¹² S. Komar Kawatra, Timothy C. Eisele, "Coal Desulfurization, High-Efficiency Preparation Methods". Page 334.

both organic and pyritic coal resulting in sulfur removal yields in excess of 90%. A downside to this method however, is its high operating (Diver, Fluidized Oxydesulfurization of Coal, US Patent # 5529587)

Caustic Treatments

Caustic treatments are yet another possibility for desulfurizing coal. Strong alkalis can be used to remove both organic and inorganic sulfur components of coal, so investigations into aqueous base leaching, microwave desulfurization, and molten caustic leaching were explored.

Battelle Hydrothermal Coal Process

Aqueous base leaching, a process ran under Battelle Hydrothermal Coal Process, involves grinding coal members and mixing the particles with an aqueous solution of 10% NaOH and 2-3% Ca(OH)₂. This mixture is then autoclaved for 10-30 minutes at temperatures ranging from 250-350°C, with subjective pressures of 2500 psi. After autoclaving, the leachant is removed and the desulfurized coal is left to dry, while the leachant can be recovered after treatment with CO₂ and lime¹³. This method can reduce the ash content of coal from 98% to 0.7%¹⁴ and removes between 90-99% of pyrite and 70% of organic sulfur, leaving a general heating value loss of 10%²⁸. However, corrosion can pose a dilemma when using alkaline solutions such high temperatures. The general process is also expensive, since the coal must be ground and autoclaved, making the process hard to implement.

Microwave desulfurization

Microwave desulfurization bases off the ability of raising the temperature of the coal at a very rapid rate such that heat activates regions of coal with high sulfur content to a point where they will react readily with NaOH. With this process, coal must be ground to fine particles (as small as 600 μm) and blended into an aqueous solution of sodium hydroxide and water. The coal is then microwaved for a few minutes while holding a 1:1 ratio of coal to NaOH. Norton et. al. experimented with Microwave desulfurization in Illinois No. 6 coal, and after three treatments found a reduction of sulfur by 83%, along with an ash reduction of 87%²⁸. Using microwave desulfurization is a potential method for

¹³ Kawatra, S. and Eisele, T. *Coal Desulfurization- High Efficiency Preparation Methods*. Taylor and Francis, New York. 2001.

Norton, G.A., Bluhm, D.D., Markuszewski, R., and Chriswell, C.D. "Application of Microwave Energy to Caustic Cleaning of Coal."

Processing and Utilization of High-Sulfur Coals IV. Elsevier, Amsterdam, pp. 425-438. 1991.

¹⁴ Balaz, P., LaCount, R.B., Kern, D.G., and Turcaniova, L. "Chemical Treatment of Coal by Grinding and Aqueous Caustic Leaching." *Fuel*. Elsevier, Amsterdam, pp. 665-671. 2001.
Meyers, R.A. *Coal Desulfurization*. Marcel Dekker, New York. 1977.

this project, however the expense per unit required for microwaving causes issues in long term implementation.

Molten Caustic Leaching (MCL)

Molten caustic leaching (MCL), a method implementing sulfur removal with strong bases at high temperatures, appears to give an effective route for removing sulfur from coal. Using molten NaOH with coal at 150°C releases pyritic sulfur, and when subjected to temperatures over 200°C organic sulfur is released. Leaching the coal with molten NaOH and KOH for 60-180 minutes at 370-400°C successfully removes 90-95% pyritic sulfur, 70-90% organic sulfur, and 90-99% of ash content. MCL has three different variations. The first method uses a mixture of molten KOH and NaOH as general alkalis to remove the sulfur. During recent experiments at Ames Laboratory in Iowa, medium-rank coals were found to have sulfur effectively removed at temperatures below 350° when leached with both KOH and NaOH. Above this temperature, however, NaOH can be used as the sole leaching agent. For high-rank coals, effective results were recorded when KOH and NaOH were used in conjunction¹⁵. The next method, known as the Gravimelt process, heats 2.5 parts anhydrous NaOH with 1 part pulverized dry coal at 400°C for 1-2 hours. The coal and NaOH is then rinsed with 2-10 parts water in a counter-current flow. Lastly the coal is flushed with H₂SO₄, rinsed with water, and then dried. This method removes over 90% of ash and both organic and inorganic sulfur from bituminous and brown coals. The last method involves washing the coal in boiling water bath for one hour and using a float/sink separation to remove sulfur in a 50% solution of NaOH. Afterward, the coal/NaOH mixture is heated for 15 minutes at 390°C. With this method a 1:1 ratio of NaOH to coal can be used that yields results similar to prior methods²⁹.

An advantage of Molten Caustic Leaching is the creation of volatile side-products. These volatiles can be separated and remarketed as fuels themselves because of their high percentage of combustible materials. However, this loss of volatile materials from the coal member does make the MCL coal harder to ignite. The resulting coal burns it does burn in a comparable fashion to the pre-treated coal. The differences created in the coal structure after leaching (e.g. a higher Na₂O content) could cause slagging or fouling, however, the benefit of low sulfur content prevails.

¹⁵ *Processing and Utilization of High-Sulfur Coals IV*. Elsevier, Amsterdam, pp. 425-438. 1991.

Balaz, P., LaCount, R.B., Kern, D.G., and Turcaniova, L. "Chemical Treatment of Coal by Grinding and Aqueous Caustic Leaching." *Fuel*. Elsevier, Amsterdam, pp. 665-671. 2001.

Meyers, R.A. *Coal Desulfurization*. Marcel Dekker, New York. 1977.

3. Physical Methods

There are numerous physical methods by which coal can be desulfurized prior to combustion. While physical methods act exclusively on inorganic forms of sulfur in coal, they tend to be far more economical than their chemical or biological counterparts. Physical methods researched primarily in this paper include: Oil Agglomeration, Froth Flotation, High Gradient Magnetic Separation, Jigs & Air Classifiers, Gravity Separation, and certain combinations of the previously mentioned methods. In the review of these particular methods special attention needs to be paid to weight yield, pyrite removal, ash removal, as well as economic factors such as equipment and utility costs.

Jigs/Air Classifiers

Jigs and air classifiers are perhaps the most economic of physical method, since they use only air/water and compressors/pumps. They also have the added advantage of a high processing capacity of up to 1000 tons per hour. To start, air classifiers use bursts of air to separate coarse members from more finely ground coal particles. A float-sink analysis can then be performed on the coarse particles to remove pyrite from coal. Major tests conducted by the EPA showed the reduction of pyritic sulfur to be in the range of 20.1-51.7% for BCR-Majac unit of air classifier, and 16.6-33.1% for the Alpine Zigzag air classifier. It is important to note that data for the Majac unit was conducted over 10 different types of coal while the Zigzag was used on only one type. (Eliot)

Jigs such as the Baum, Pan-American Placer, and Batac are in commercial use and provide considerable results. Jigs utilize fluids such as air or water in a pulsating, typically sinusoidal, pattern in an effort to stratify and separate coal and pyrite based on density differences. The Baum and Batac Jigs use primarily air in their process, as opposed to the Pan-American Jig that uses water. While structurally similar, the main discerning factor that separates the Baum Jig from the Pan-American Jig is that the Baum Jig emphasizes the pulsing stroke whereas in the Pan-American Jig, implements a suction stroke is equally important. The Batac Jig, in tests performed by Hoke in 1976, showed distinct advantages over the Baum Jig. This form of Jigs not only has the capability of handling smaller particle sizes, but also yields a better recovery for combustible material (95.7-97.0% vs 83.7-88.0%). In terms of coal cleaning abilities, the Baum Jig showed pyrite removal in the 53.2-68.2% and ash removal in the 88.0-91.0% range, while the Batac ranged in the 56.6-61.3 % and 67.6-79.8%, respectively. Combinations of Baum and Batac Jigs would increase particle size range, and yield approximated pyrite removal in the 40-89% range. (Kawatra & Eisele)

While Jigs has the advantage of being an economical choice, their ability to remove sulfur from coal is fairly limited. Jigs could potentially be used in conjunction with other methods, however due to the larger particle size necessary for the use of Jigs, an intermediate pulverizing stage subsequent to Jigs would be necessary for other methods to process.

Gravity Separation

The dry method of gravity separation is primarily known as the dry table. This process uses an oscillating incline to separate pyrite from coal by gravitational means. Much like the Jig systems, dry tables use larger particle sizes and produce limited results.

The wet method of gravity separation is a sink-float test conducted within a heavy liquid with specific gravities nearing 1.4-1.6. These liquids are typically chlorinated or brominated hydrocarbons, though zinc chloride water has also been implemented for use. While the effectiveness of gravity separations is widely available in literature, it is not a recommended method. This is due to the high costs of brominated and chlorinated liquids and their ability to contaminate groundwater, air, and even alter the coking properties of coal. For these reasons, gravity separation is not a desirable process for this IPRO. (Wheelock)

Oil Agglomeration

Oil agglomeration is the method of adding fuel oils to coal slurry. Addition of fuel oil causes the coal particles in solution to agglomerate and float to the top, while impurities such as pyrite and ash remain in solution. While literature has cited oil agglomeration as a useful method for the desulfurization of coal, the added costs of large amounts of fuel oils for a large scale process would be economically unfeasible. The fact that all literature found regarding this process were bench-scale lends credence to that theory. (Eliot)

Froth Flotation

Flotation and Froth Flotation are a couple of the more standard physical processes used within industry. Flotation exploits the density properties of coal and pyrite relative to water. Coal is less dense than water and is able to retain at the top, while ash and pyrite sink to the bottom. Froth Flotation, on the other hand, uses a chemical treatment to create a hydrophobic & hydrophilic relationship between coal & pyrite. Hydrophobic coal in the presence of a frothing agent and gas bubbling causes adherence, hence forcing coal to float to the top. Hydrophilic pyrite and ash become heavy and sink. Flotation and Froth Flotation require raw coal be ground finely for best results. However, finely ground pyrite might also float to the top in some instances. As a result, a two-stage process patented by the Mining Bureau uses the typical method of froth flotation for the first stage, where coal is the top product and pyrite the bottom. In the second stage, the top of the first stage are concentrated, fresh water is added, and a flotation suppressant added; resulting in the coal becoming the bottom product of the second stage. Testing of flotation, froth flotation, and two stage froth flotation show it to be effective in eliminating significant portions of both pyrite and ash content in coal with reasonable recovery of flammable materials. (Wheelock) (Eliot)

High Gradient Magnetic Separation

Magnetic separation is a technique previously used for the purification of kaolin clay. It has recently been applied to coal desulfurization, based on the differing magnetic properties of coal and pyrite. In this process, a finely ground coal slurry solution is run through a magnet wrapped in steel or stainless steel wool. Pyrite and ash are attracted to the steel wool while coal is allowed to pass through. Treatment with steam was originally thought to enhance the magnetic properties of coal, but recent chemical treatments show to be more effective. When treated, coal particles will be repelled by the magnets, while ash and pyrite are strongly attracted to them. Studies show high gradient magnetic separation to be effective at eliminating up to 90% of pyritic sulfur with up to 95% recovery of flammable materials. One of the main disadvantages of the magnetic method is the necessary downtime to backwash the magnets to prevent pyrite build-up. However, more recent technology has created a rotating carousel magnetic that can be used continuously. This leaves the only major disadvantage of magnetic separation to be the cost of electricity necessary to power the magnets, which relative to other methods, is extremely high. (Wheelock)

Heavy Media Vessels

Heavy media processes take advantage of the fact of coal's lower specific gravity than its impurities. If a liquid which has a specific gravity between that of coal and that of the impurities (a so-called 'heavy-liquid') is added to ground coal, the lighter coal particles will float, while the heavier impurities will sink. Performing the process in a cyclone gives better cleaning efficiency than an agitated pool. In full scale plant (Kawatra et al., 1995), a heavy media bath gave a pyritic sulfur removal of 68%. This method shows great resemblance to the floatation method previously discussed. (Kawatra and Eisele)

Heavy Media Cyclones

Heavy media separations in cyclones allow extra force, in addition to the gravitational force, when separating coal members. When this is implemented to other processes, separation efficiencies tend to increase. In addition, due to their design, these cyclones can process a much finer particle size than other separators. The most commonly used media in heavy media cyclone are standard magnetic media, true heavy liquids, micronized magnetite, magnetic fluids, and pure water only. (Kawatra and Eisele)

Standard Magnetic Media

The advantage to magnetic media is that it is easily recovered by magnetic separation, reducing operating cost. In a full scale plant (Kawatra et al., 1995), a heavy media cyclone using standard magnetic media yielded a sulfur

removal of 55.6% with a recovery of 56.32 weight %. One drawback of this process is that the magnetite is also removed by the centrifugal force of the cyclone, reducing separation efficiency. (Kawatra and Eisele)

True Heavy Liquids: True heavy liquids such as perchloroethylene, carbon tetrachloride, broomcorn, and tetrabromoethane will not settle out of the solution with time making them preferred. This means that it is not necessary to constantly agitate them to prevent settling. A disadvantage however, lies in their expense and toxicity. (Kawatra and Eisele)

Micronized Magnetite: Grinding magnetite to a very fine particle size (90% finer than 7 micrometers) has two main advantages over standard magnetic media. First, this makes the solution less likely to settle over time, and as a result, smaller diameter cyclones can be utilized (Kawatra and Eisele, p. 84). Its separating efficiency for very fine particles is similar to that of standard magnetic media cyclones for coarser particles, allowing this method to give greater accuracy.

Magnetic Fluids: Units using the magnetic fluid principle in combination with centrifugal forces have been marketed both on a laboratory and a pilot plant scale, but the equipment needed for a full-scale plant installation is still under development. Once such a unit has been developed, its separating efficiency should equal if not exceed that of true heavy liquid separators. (Kawatra and Eisele, p. 85)

Water-Only: The main advantage to water-only cyclones are the simplicity and economical aspects of installation and operation. High separation efficiencies are not as common as competing processes, so they are best used as a pre-cleaning stage for subsequent separation process. At an industrial-scale, a water only cyclone provided a separation efficiency of 70-80% for particles greater than 600 by 150 micrometers, with corresponding decreases in separation as particle size decreased. (Kawatra and Eisele, p. 86)

Decanter Centrifuge: The advantage to a decanter centrifuge is its ability to produce greater centrifugal forces than conventional cyclones. For this reason, it can use heavy liquids that are more viscous, and can't be implemented in conventional cyclones. Since these are generally less toxic than the true heavy liquids used in conventional cyclones, cleanup after an accident would cost significantly less. The disadvantage to a decanter centrifuge lies in its high operating cost compared to other cyclones. (Kawatra and Eisele, p. 88)

Flowing Film Concentrators

Flowing film concentrators use a flowing film moving across a surface to separate out impurities. Since coal is less dense than its impurities, it is less affected by gravity and more affected by the velocity of the fluid. Conversely, the denser impurities are played off the gravity aspect of this mechanism. As a result, the lighter coal particles are generally displaced to the outside of the film, while the impurities remain mostly un-displaced. Since the method relies on the strength of gravitational forces, larger (and therefore heavier) coal particles will end up in the same place as much smaller (and lighter) particles of impurities. For this reason, flowing film concentrators work best if the feed has been prescreened for size.

Tables: Jets of water are streamed across a table which is being shaken laterally. Denser particles are more affected by the shaking of the table, while less dense particles are more affected by the flow of the water. Efficiencies of 99% sulfur removal have been claimed, when subjected to coal containing 17.51% sulfur. (Kawatra and Eisele, p. 100)

Spirals: A stream of water is run down a spiraling chute. Fluid forces cause the less dense coal particles to move to the outside of the chute, while the more dense particles remain near the inside. Some advantages of spirals are that they are easy and cheap to install, operate, and maintain, and that they take up relatively little floorspace for a given capacity. On a test scale, the sulfur removal of a spiral was found to be 85%. (Kawtra and Eisele, p. 104)

Hidered Bed Separators

Hindered bed separators use an upward flowing fluid to separate coal from its impurities. As in flowing film concentrators, fluid forces affect the less dense coal particles more strongly than the more dense impurities. The less dense particles remain at the top of the fluid and are carried off by the overflow, while the more dense particles sink to the bottom where they carried off as reject product. The advantage to hindered bed separators are low cost and simple operation. It has also been shown that they have slightly better separation efficiency than spirals at certain ranges of particle size. (Kawatra and Eisele, p. 107)

Packed and Baffled Columns

Column flotation, in which hydrophobic coal attaches to froth bubbles to rise to the top of the liquid, can be improved by adding packing or baffling to the column.

Packing: Adding corrugated plates with only very small spaces between the packing greatly reduces the size of the bubbles, thus increasing the total surface area. The disadvantage to adding packing to the column is

that if particles larger than the channels between the packing are present, they can abrade and plug the packing. Additionally, the froth at the top of the machine can dry out and plug the column, making constant wetting of the froth necessary. On a laboratory scale, a packed column was found to have 57.3% sulfur removal.

Baffling: Adding baffles to the column gives many of the advantages of adding packing while avoiding the accompanying problems. Baffles reduce the bubble size, allowing more surface area for coal, while still allowing for coarse particles to travel short distances, avoiding the plugging problem. Additionally, if baffles are installed below the feed inlet, they can increase the mean residence time in the column, increasing separation efficiency. One of the largest advantages of baffles is that they are cheap and can be retrofitted onto existing froth flotation columns. On an industrial scale, baffled columns provided between 51.7% (for 85.26% energy recovery) to 94.6% (for 18.19 % energy recovery) pyritic sulfur removal. (Kawatra and Eisele, p. 203)

Selective Agglomeration

Like froth flotation, selective agglomeration takes advantage of coal's hydrophobic nature to produce separation. The main difference is that instead of bubbles, the coal particles attach to immiscible oils upon agitation. Some agglomerants that have been suggested are fuel oils, n-chain hydrocarbons, liquid carbon dioxide, and chlorofluorocarbons. The main disadvantage to the process is that the high usage of agglomerant results in relatively high operating costs. Since selective agglomeration's efficiency is no better than that of froth flotation (50-80 % pyritic sulfur removal), separating efficiency doesn't justify the extra cost created by this process. However, if a high energy yield fuel is used as the agglomerant, it can be left in and burned along with the clean coal, eliminating the need to dry the coal after cleaning. (Kawatra and Eisele, p. 237)

Wheelock, Thomas D. Coal Desulfurization: Chemical and Physical Methods. American Chemical Society: 1977
Demirbaş, A. & Balat, M. "Coal Desulfurization Via Different Methods". *Energy Sources*, 26: p.541-550. Taylor & Francis, Inc. 2004
Sutcu, Hale. "Coal Desulfurization Using Natural Ca-Based Sorbents". *Coal Preparation*, 24: p.249-259. Taylor & Francis, Inc. 2004
Eliot, Robert C. Coal Desulfurization Prior to Combustion. Noyes Data Corporation: 1978

Assignments

IPRO 346 was dispersed into the following groups throughout the semester. The groups changed very little from the midterm of the project.

Coal Research Group

Tony Doellman
Gregg Kisiel
Myint Toe

Coke Research Group

Salil Benegal
Amy McDowell
Oscar Olmos

Desulfurization and Coal Analysis Group

Andrew Keen
James Maratt
Adejoke Ogunrinde

Physical Methods Group

Tony Doellman
Andrew Keen
Adejoke Ogunrinde

Chemical Methods Group

Salil Benegal
James Maratt
Amy McDowell
Oscar Olmos

Biological Methods Group

Gregg Kisiel
Myint Toe

Process Design Group Analysis Group

Amy McDowell
James Maratt
Oscar Olmos
Andrew Keen

Costing and Profitability

Adejoke Ogunrinde

Safety Group

Greggory Kisiel

Assignments have also been given for some of the particulars of this IPRO:

- Project Plan – Team Leader in collaboration with members and advisor
- Research – All Team Members
- Oral Presentation – Amy McDowell, James Maratt, Oscar Olmos, Adejoke Ogunrinde, Greggory Kisiel
- Midterm Progress Report – Team Leader in collaboration with members and advisor
- Team Minutes - Adejoke Ogunrinde
- Team Poster – James Maratt, Oscar Olmos, Amy McDowell
- Final Report/Abstract – Team Leader in collaboration with members and advisor
- Collection and Summary of Weekly Time Sheets – James Maratt
- Weekly Tasks – Oscar Olmos
- iKnow/ iGroups Coordinator- Amy McDowell

Obstacles

A few obstacles were encountered with this project. The decision making process for a desulfurization method took longer than expected. Also, our work was delayed due to team members' other obligations with other classes and work. While deadlines set were reasonable, some of them overlapped with other priorities (e.g. midterm exams, term papers) and were not always met. Last, this IPRO was challenging due to the type of problem faced. After initial research was completed, it was difficult to assign tasks for students without a chemical engineering background. Much work needed to be done to model our process, and the extended period of time needed for this task caused other members of the team to wait until it was finished for something more to do. Many of our project tasks were linked together, therefore some had to be completed before others could be assigned.

Results

While initially we hit a road block modelling our chosen method, eventually we succeeded using semi-unorthodox methods. While modelling using Hysys, ChemCad or a number of other computer simulation programs is a more traditional and easy method for our task we instead modelled our reactors by hand calculations and ODE solvers. These methods presumably give the same results, however the simulations programs that we had on hand would not model solids.

Our group determined that oxydesulfurization was a fitting method for this project. The total amount of sulfur removed was 86%, which was above the limit of 81% set by the EPA. We were able to remove 95% of pyritic sulfur along with 72% of organic sulfur. An incoming feed of 70 tons/hr leads to a total of 2080kg of sulfur removed per hour (total sulfur before removal amounting to 2416kg).

The following calculations were performed in our process.

EPA maximum SO₂ allowed

The Environmental Protection Agency (EPA) states that the maximum SO₂ allowed should be:

$$\frac{2.5 \text{ lb SO}_2}{1 \times 10^6 \text{ BTU}} \text{ produced.}$$

This means that for your Illinois #6 coal:

$$0.23388 \frac{\text{kmol}}{\text{m}^3} \text{ SO}_2 * 64 \frac{\text{Kg SO}_2}{\text{kmol SO}_2} = 14.96 \frac{\text{kg SO}_2}{\text{m}^3} * 100 \text{ m}^3 = 1496 \text{ kg SO}_2$$

$$1496 \text{ kg SO}_2 = 3298.11 \text{ lb SO}_2 \text{ Produced per hour.}$$

$1768 \frac{BTU}{lb} = 2.475 \times 10^8 BTU * 2.5 \frac{lbSO_2}{1 \times 10^6 BTU} = 618.75 lbSO_2$ Allowed per 70 tons of coke.

$$100 - \frac{618.75 lbSO_2}{3298.11 lb} * 100 = 81.23\%$$

This means that our coal should be desulfurized at least 81.23% in order to meet EPA standards.

Amount of Various Types of Sulfur in Coal:

$$70 tons * \frac{907 kg}{ton} * \frac{0.175}{100} = 111.10 kgS$$

$$70 tons * \frac{907 kg}{ton} * \frac{1.825}{100} = 1158.69 kgPyritic$$

$$70 tons * \frac{907 kg}{ton} * \frac{1.805}{100} = 1145.99 kgOrganic$$

$$111.1 + 1158.69 + 1145.99 = 2415.78 kg$$

$$111.10 kgS * .9465 = 105.2 kgS$$

$$1158.69 kgPyritic * .995 = 1152.9 kgPyritic$$

$$1145.99 kgOrganic * .9465 = 822 kgOrganic$$

$$105.2 + 1152.9 + 822 = 2080.1 kgTotalSulfur$$

$$\frac{2080.1 kgSO_2}{2415.78 kg} * 100 = 86.1\%$$

Total sulfur removed is 86.1%.

Main Reactor Design

Our process is best utilized by using the Kunii-Levenspiel bubbling-bed model to explain what is happening in our fluidized bed. This model's technique begins with the reactant gas entering the bottom of the fluidized bed and flowing up in the form of bubbles through the reactor vessel. Mass transfer occurs among the gases as they diffuse between the bubbles and come in contact with the solid particles, where the reaction product is formed. The product then flows back into a bubble and finally exits the bed when the bubble reaches the top of the bed. The rate at which the reactants and products transfer in and out of the bubble affects the conversion, as does the time it takes for the bubble to pass through the bed. Consequently, we need to describe the velocity at which the bubbles move through the column and the rate of transport of gases in and out of the bubbles. To calculate these parameters we need to determine a number of fluid-mechanics parameters associated with the fluidization process. Specifically, to determine the velocity of the bubble through the bed: Minimum fluidization velocity, U_{mf} and also the diameter of the solid d_b .

$$U_{mf} = \frac{\mu Re_{mf}}{\rho_f d_p} \quad (1)$$

$$Re = (1135.7 + 0.0408 * Ar)^{0.5} - 33.7$$

$$Ar = \frac{d_p^3 \rho_f (\rho_s - \rho_f) g}{\mu^2} \quad (2)$$

$$Ar = \frac{0.0047625^3 * 10.581(716 - 10.581) * 9.8}{2.7346E - 5^2} = 10566162.6 \quad (3)$$

$$Re = (1135.7 + 0.0408 * 10566162.6)^{0.5} - 33.7 = 623.74$$

$$U_{mf} = \frac{2.7346 \times 10^{-5} * 623.74}{10.581 \frac{kg}{m^3} * 0.0047625m} = 0.33 \frac{m}{s} = 33 \frac{cm}{s} \quad (4)$$

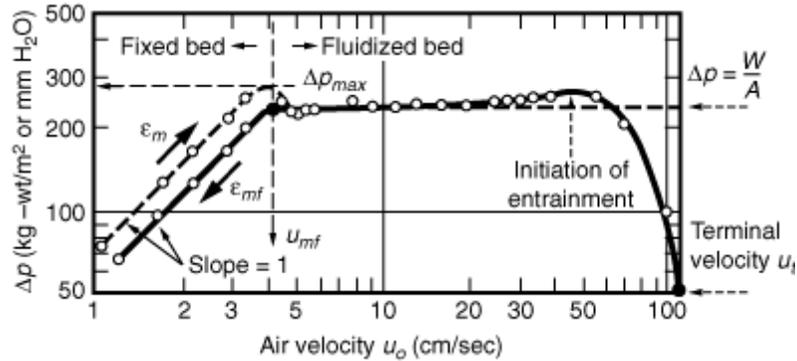
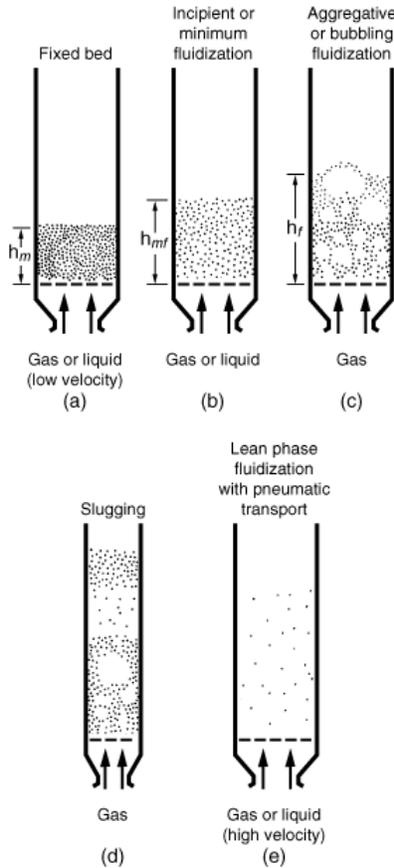


Diagram 1: Minimum Fluidization Velocity

The minimum fluidization velocity turns out to be 33cm/s, and as we can see, by literature the terminal velocity is around 50cm/s.

If the gas velocity is increased still further, expansion of the bed will continue to occur; the solid particles will become somewhat separated from each other and begin to jostle each other and move around in a restless manner. Increasing the velocity just a slight amount causes further instabilities and some of the gas starts bypassing the rest of the bed in the form of bubbles (Figure 1). Coincidentally with this, the solids in the bed begin moving upward appearing as a boiling frothing mixture. With part of the gas bubbling through the bed and the solids being moved around as though they were part of the fluid, the bed of particles is said to be *fluidized*. Finally, at extremely high velocities the particles are blown or transported out of the bed (Figure 1e).



17
Figure 1:

Next step is the calculation of the ΔP . Assuming a height equal to 8m.

$$\frac{\Delta P}{h} = \rho_g U^2 \left[\frac{150(1 - \epsilon)}{Re_d \psi} + \frac{7}{4} \right] \frac{1 - \epsilon}{\psi d_p \epsilon^3} \tag{5}$$

$$\Delta P = 8m * 10.281 \frac{kg}{m^3} * 0.33^2 * \left[\frac{150 * (1 - 0.63)}{623.74 * 0.52} + \frac{7}{4} \right] \frac{1 - 0.63}{0.52 * 0.0047625 * 0.63^3} = 10281.3 Pa = 1.49 psi$$

(6)

Now, we need to calculate the cross sectional area:

The weight of the bed is $W=70$ tons.

$$A = 70ton * \frac{1}{10281.3 pa} * \frac{907kg}{1ton} * 9.8 \frac{m}{s^2} = 60.59m^2 \tag{7}$$

In order to insure a safely running fluidized bed, we decided to increase the area of our vessel by 10%.

¹⁷ Fogler. “Elements of Chemical Reaction Engineering”, 4th Edition.

$$A = \pi r^2 l$$

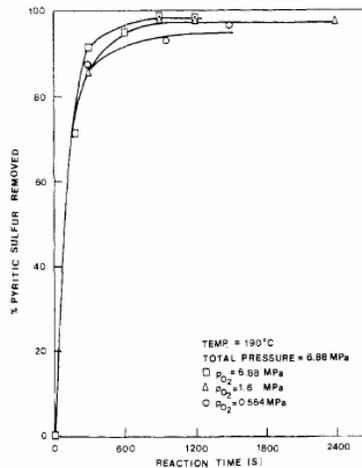
$$r = \sqrt{\frac{66.72}{3.1415}} = 4.6084m \quad (8)$$

$$V = A * l = 533.76m^3 \quad (9)$$

Kinetics Calculations

For the following reactions:

- Assume oxygen in excess and pyritic sulfur as limit reactant.
- Isothermal reactor is assumed
- Reactor conditions:
 - T=260°C+273.15=533.15K
 - P=8MPa overall
 - P_o=1.6Mpa
- CSTR, and Batch reactors were modelled
- A reaction time of 1800 seconds (30 minutes) suggested by literature (Graph 1)



Graph 1: Experimental sulfur removal vs Reaction Time.

A. Pyritic Sulfur

Second order rate of reaction dependent only in concentration of sulfur.

$$\frac{dC_{ps}}{dt} = -K_p C_s^2 \quad (10)$$

$$K_p = 1.14 \times 10^4 \cdot \exp \left[\frac{-46.5 \times 10^6 \frac{J}{kmol}}{RT} \right] \quad \left[\frac{m^3}{kmol \cdot s} \right] \quad (11)$$

$$R = 8.3144 \frac{J}{mol \cdot K} = 8314.4 \frac{J}{Kmol}$$

B. Oxydation of Carbon

$$\frac{dC_c}{dt} = -K_0 \quad (12)$$

Zero order rate of reaction

$$K_0 = 1.469 \times 10^7 \exp \left[\frac{-85.5 \times 10^6 \frac{J}{kmol}}{RT} \right] \quad \left[\frac{mol}{m^3 \cdot s} \right] \quad (13)$$

C. Organic Sulfur

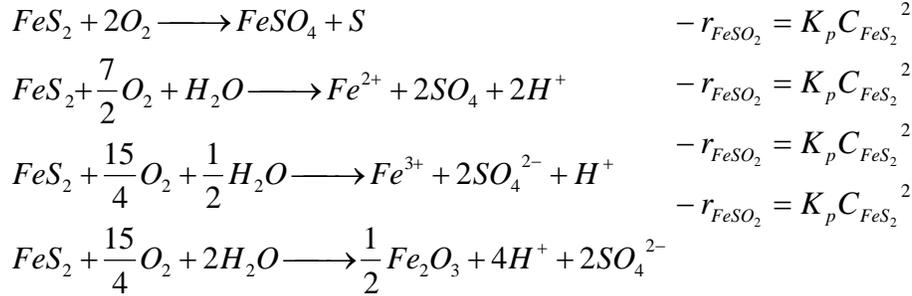
$$\frac{dW_{os}}{dt} = -K_o \quad (14)$$

Zero order rate of reaction

$$K_o = 2.1 \times 10^2 \exp \left[\frac{-78.5 \times 10^6 \frac{J}{kmol}}{RT} \right] \quad \left[\frac{kgS}{kgcoal \cdot s} \right] \quad (15)$$

Reactions in Fluidized Reactor

A. Pyritic Sulfur



Relationship between reactants:

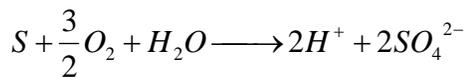
$$1. \quad \frac{r_{1FeS_2}}{(-1)} = \frac{r_{1O_2}}{(-2)} = \frac{r_{1FeSO_4}}{(1)} = \frac{r_{1S}}{(1)} \quad (16)$$

$$2. \quad \frac{r_{2FeS_2}}{(-1)} = \frac{r_{2O_2}}{(-\frac{7}{2})} = \frac{r_{2H_2O}}{(-1)} = \frac{r_{2Fe^{2+}}}{(1)} = \frac{r_{2SO_4^{2-}}}{(2)} = \frac{r_{2H^+}}{(2)} \quad (17)$$

$$3. \quad \frac{r_{3FeS_2}}{(-1)} = \frac{r_{3O_2}}{(-\frac{15}{4})} = \frac{r_{3H_2O}}{(-\frac{1}{2})} = \frac{r_{3Fe^{3+}}}{(1)} = \frac{r_{3SO_4^{2-}}}{2} = \frac{r_{3H^+}}{1} \quad (18)$$

$$4. \quad \frac{r_{4FeS_2}}{-1} = \frac{r_{4O_2}}{-\frac{15}{4}} = \frac{r_{4H_2O}}{-2} = \frac{r_{4Fe_2O_3}}{\frac{1}{2}} = \frac{r_{4H^+}}{4} = \frac{r_{4SO_4^{2-}}}{2} \quad (19)$$

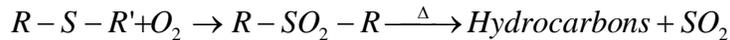
B. Elemental Sulfur



$$r_{FeS_2} = \sum_{i=1}^4 r_{iFeS_2} = -4K_p C_{FeS} \quad (20)$$

$$5. \quad \frac{r_{5S}}{-1} = \frac{r_{5O_2}}{-\frac{3}{2}} = \frac{r_{5H_2O}}{-1} = \frac{r_{5H^+}}{2} = \frac{r_{5SO_4^{2-}}}{2} \quad (21)$$

C. Organic Sulfur



D. Limestone neutralization Reaction



CSTR and Batch Models

All of the reactions in the CSTR will be modeled as liquid phase reaction.

$$C_j = \frac{F_j}{V_o} \tag{22}$$

V_o = volumetric flow rate of the reactants. This is:

$$\text{Volume of coal: } 70 \frac{\text{ton}}{\text{hr}} * 907 \frac{\text{kg}}{\text{ton}} * \frac{1 \text{m}^3}{716 \text{kg}} = 88.67 \frac{\text{m}^3}{\text{h}} \tag{23}$$

Volume of air+steam: Calculating in Aspen with Peng-Robinson equation, 50% air, 50% water mixture: A total of $14.5 \frac{\text{kmol}O_2}{\text{hr}}$ is needed for reactions 1-4 per 4kmol of pyritic sulfur reacted.

Volume of Reactants: $5 \frac{\text{m}^3}{\text{hr}}$ @ 8MPa, 533K

Total reactants volume is:

$$V \cong 100 \frac{\text{m}^3}{\text{hr}} \tag{24}$$

Pyritic Sulfur

Modeling the reactor with a continuous flow rate of 70ton/hr of coal.

Since, $r_{FeS_2} = \sum_{i=1}^4 r_{i_{FeS_2}} = -4K_p C_{FeS}$ we calculate the “molar flow rate” as:

Molecular Weight of FeS_2 (pyritic sulfur):

Fe = 55g/mol

S = 32g/mol

Initial Pyritic concentration $FeS_2 = 119 \frac{\text{g}}{\text{mol}}$

From table 1:

$$\text{Totalmols}_{FeS_2} = 70\text{tons} * 907.1 \frac{\text{kg}}{\text{ton}} * 0.01825 * \frac{1\text{kmol}}{119\text{kg}} = 9.73\text{kmol} \quad (25)$$

$$r_{FeS_2} = \sum_{i=1}^4 r_{i_{FeS_2}} = -4K_p C_{FeS_2}$$

1. As a batch reactor Model:

$$\frac{dC_{FeS_2}}{dt} = -4 * (0.3170) * C_{FeS_2}^2$$

$$\int \frac{1}{C_{FeS_2}^2} dC_{FeS_2} = \int -4 * (0.3170) dt$$

$$\frac{-1}{C_{1FeS_2}} + \frac{1}{C_{0FeS_2}} = -4 * (0.3170) * 1800$$

$$C_{0FeS_2} = \frac{9.73\text{kmol}}{100\text{m}^3} = 0.0973 \frac{\text{kmol}}{\text{m}^3}$$

$$C_{1FeS_2} = 4.3813 \times 10^{-4} \frac{\text{kmol}}{\text{m}^3}$$

$$\% \text{Pyriticsulfurleft} = \frac{4.3813 \times 10^{-4} \frac{\text{kmol}}{\text{m}^3}}{0.0973 \frac{\text{kmol}}{\text{m}^3}} * 100 = 0.4522\%$$

$$\% \text{desulfurizationpyritic} = 100 - 0.4522 = 99.5\% \quad (26)$$

2. As CSTR:

$$V = V_0 * \frac{C_{0_{FeS_2}} - C_{FeS_2}}{-r_{FeS_2}} \quad (27)$$

$$V = 533.76\text{m}^3$$

$$V_0 = 100 \frac{\text{m}^3}{\text{hr}} * \frac{1\text{hr}}{3600\text{s}} = 2.77\text{E} - 2 \frac{\text{m}^3}{\text{s}}$$

$$C_{0_{FeS_2}} = 0.0973 \frac{\text{kmol}}{\text{m}^3}$$

Solving for $C_{FeS_2} = 3.91 \times 10^{-3} \frac{\text{kmol}}{\text{m}^3}$

$$\% \text{Pyritic sulfur left} = \frac{3.91 \times 10^{-3} \frac{\text{kmol}}{\text{m}^3}}{0.0973 \frac{\text{kmol}}{\text{m}^3}} * 100 = 4.0184\% \quad (28)$$

$$\% \text{desulfurization pyritic} = 100 - 4.0184 = 95.98\% \quad (29)$$

Oxidation of Carbon

1. Batch Reactor

$$\frac{dC_c}{dt} = -(K_0)$$

$$\frac{dC_c}{dt} = -(1.69)$$

$$\int dC_c = \int -(1.69) dt$$

$$C_{1c} - C_{0c} = -(1.69 \frac{\text{mol}}{\text{m}^3 \text{s}}) * 1800 \text{s}$$

$$70 \frac{\text{tons}}{\text{ton}} * 907.1 \frac{\text{kg}}{\text{ton}} * 0.6547 * \frac{1 \text{ kmol}}{12 \text{ kg}} = 3464 \frac{\text{kmol}}{\text{m}^3}$$

$$C_{0c} = \frac{3464 \text{ kmol}}{100 \text{ m}^3} = 34.64 \frac{\text{kmol}}{\text{m}^3} * 1000 \frac{\text{mol}}{\text{kmol}} = 34640 \frac{\text{mol}}{\text{m}^3}$$

Solving for the final concentration

$$C_{1c} = 34640 \frac{\text{mol}}{\text{m}^3} - 2970 \frac{\text{mol}}{\text{m}^3} = 31670 \frac{\text{mol}}{\text{m}^3}$$

$$\% \text{carbon recovered} = \frac{31670 \frac{\text{mol}}{\text{m}^3}}{34640 \frac{\text{mol}}{\text{m}^3}} * 100 = 91.42\% \quad (30)$$

2. CSTR:

$$V = V_0 * \frac{C_{0c} - C_{1c}}{-r_c}$$

$$-r_c = k = 1.69$$

$$V = 533.76m^3$$

$$C_{0c} = \frac{3464kmol}{100m^3} = 34.64 \frac{kmol}{m^3} * 1000 \frac{mol}{kmol} = 34640 \frac{mol}{m^3}$$

$$C_{0c \text{ oxidized}} = 0 \frac{mol}{m^3}$$

$$V_0 = 100 \frac{m^3}{hr} * \frac{1hr}{3600s} = 2.77 \times 10^{-2} \frac{m^3}{s}$$

Solving for $C_{1c} = 2121.22 \frac{molC_{oxidized}}{m^3}$

$$\% \text{carbonre covered} = \frac{34640 \frac{mol}{m^3} - 2121.22 \frac{molC_{oxidized}}{m^3}}{34640 \frac{mol}{m^3}} * 100 = 89.19\% \quad (31)$$

Organic Sulfur

1. Batch Reactor:

$$K = 4.2590 \times 10^{-6} \frac{kgorgS}{Kgcoal * s}$$

$$\frac{dW}{dt} = -4.2590 \times 10^{-6}$$

$$\int dw = \int -4.2590 \times 10^{-6} dt$$

Organic_sulfur

$$70 \text{toncoal} * 907 \frac{kg}{ton} * 0.01805 \text{fractionorganic} = 1145.99 \text{kgorganic}$$

$$\frac{1145.99}{70 * 907 * 0.6615} = 2.72 \times 10^{-2} \frac{kgS}{Kgcoal}$$

$$w_1 = -4.2590 \times 10^{-6} \frac{kgS}{Kgcoal * s} * 1800s + 2.72 \times 10^{-2} \frac{kgS}{Kgcoal}$$

$$w_1 = 0.01952 \frac{kgSorganic}{Kgcoal}$$

This means that the total desulfurization of organic sulfur is:

$$\%organic = \frac{0.01952}{2.72 \times 10^{-2}} * 100 = 71.76\% \quad (32)$$

2. CSTR reactor:

$$V = V_0 * \frac{W_{0org} - W_{1org}}{-r_{org}}$$

$$-r_{org} = k = 7.66 \times 10^{-3} \frac{kgorgS}{Kgcoal * s}$$

$$V = 533.76 m^3$$

Organic_sulfur

$$70 toncoal * 907 \frac{kg}{ton} * 0.01805 fractionorganic = 1145.99 kgorganic$$

$$\frac{1145.99}{70 * 907 * 0.6615} = 2.72 \times 10^{-2} \frac{kgorgS}{Kgcoal}$$

$$W_{0org} = 2.72 \times 10^{-2} \frac{kgorgS}{kgcoal}$$

$$V_0 = 100 \frac{m^3}{hr} * \frac{1hr}{3600s} = 2.77 \times 10^{-2} \frac{m^3}{s}$$

$$W_{1org} = 1.57 \times 10^{-2} \frac{kgorg}{kgcoal}$$

$$\%removal = (1 - (\frac{1.57 \times 10^{-2}}{2.72 \times 10^{-2}})) * 100 = 42.2\% removed \quad (33)$$

Rate of reactions for the rest of components modeled in polymath:

$$r_s = r_{5s} - r_{1FeS_2}$$

$$r_{5s} = -k_s C_s^2$$

$$k_s = k_p$$

$$r_{SO_4} = -r_{1FeS_2} - 2r_{2FeS_2} - 2r_{3FeS_2} - 0.5r_{4FeS_2} - 2r_{5s}$$

$$r_{H^+} = -2r_{2FeS_2} - r_{3FeS_2} - 4r_{4FeS_2} - 2r_{5s}$$

Polymath Model

Main Screen:

$k1 = 0.3170$
 $d(ca)/d(t) = -k1 * ca^2 + k1 * cb^2$
 $ca(0) = 0.034$
 $d(cd)/d(t) = 7 * k1 * cb^2 + 2 * (k1 * ca^2 - k1 * cb^2)$
 $cd(0) = 0$
 $d(cb)/d(t) = -4 * k1 * cb^2$
 $cb(0) = 0.0973$
 $d(cc)/d(t) = 7 * k1 * cb^2 + 2 * (k1 * ca^2 - k1 * cb^2)$
 $cc(0) = 0$
 $t(0) = 0$
 $t(f) = 1800$

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	t	0	0	1800.	1800.
2	ca	0.034	0.0018175	0.0348316	0.0018175
3	cd	0	0	0.2338768	0.2338768
4	cb	0.0973	0.0004362	0.0973	0.0004362
5	cc	0	0	0.2338768	0.2338768
6	ce	3.464E+04	3.16E+04	3.464E+04	3.16E+04
7	corgs	0.0272	0.0195338	0.0272	0.0195338
8	cso2	0	0	0.0076662	0.0076662
9	k1	0.317	0.317	0.317	0.317
10	k0	1.69	1.69	1.69	1.69
11	korg	4.259E-06	4.259E-06	4.259E-06	4.259E-06

Differential equations

- 1 $d(ca)/d(t) = -k1 * ca^2 + k1 * cb^2$
- 2 $d(cd)/d(t) = 7 * k1 * cb^2 + 2 * (k1 * ca^2 - k1 * cb^2)$
- 3 $d(cb)/d(t) = -4 * k1 * cb^2$
- 4 $d(cc)/d(t) = 7 * k1 * cb^2 + 2 * (k1 * ca^2 - k1 * cb^2)$
- 5 $d(ce)/d(t) = -k0$
- 6 $d(corgs)/d(t) = -korg$
- 7 $d(cso2)/d(t) = korg$

Explicit equations

- 1 $k1 = 0.3170$
- 2 $k0 = 1.69$
- 3 $korg = 4.2590E-6$

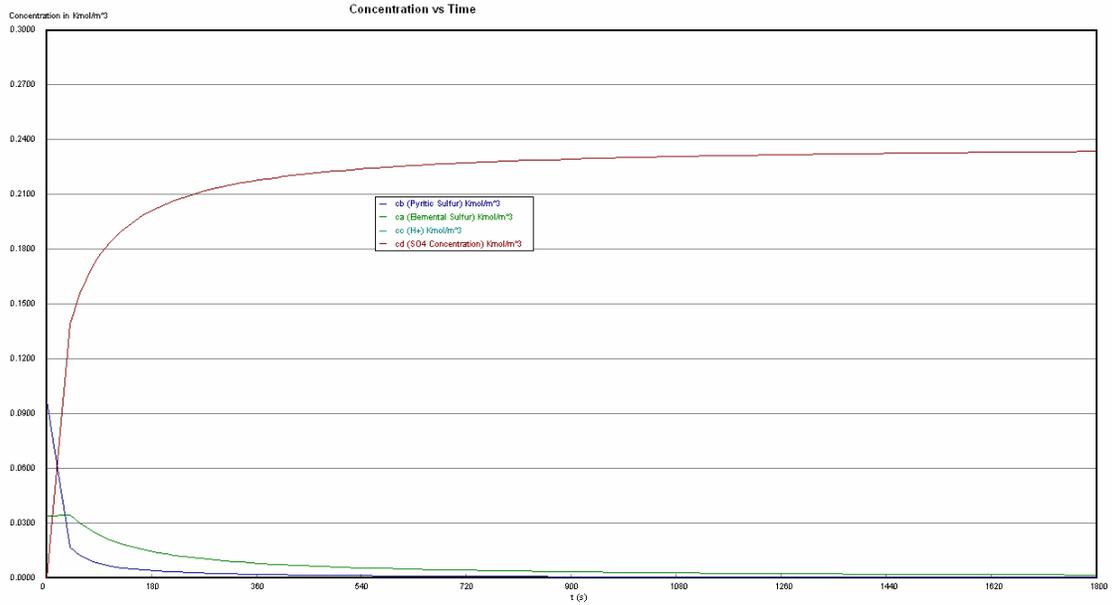


Table 4: SO_4 Production, Pyritic Reaction:

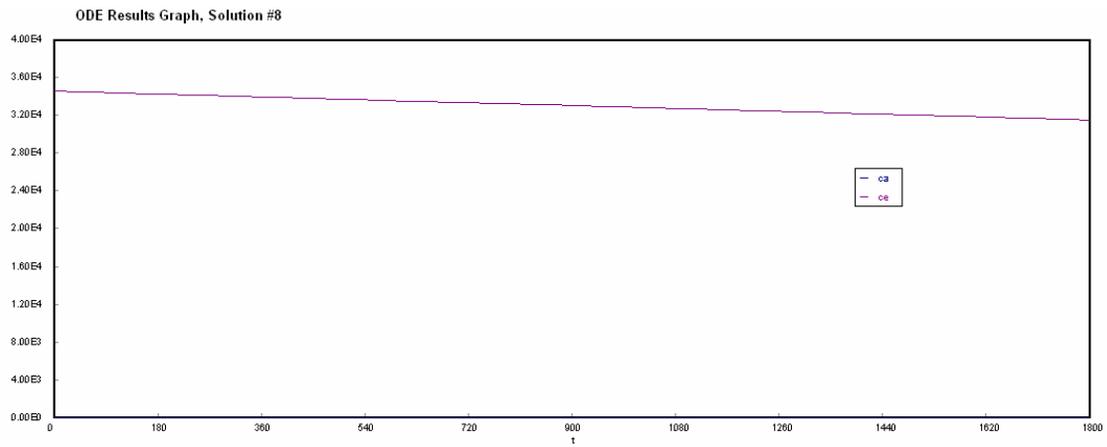


Table 5: Carbon Oxidation

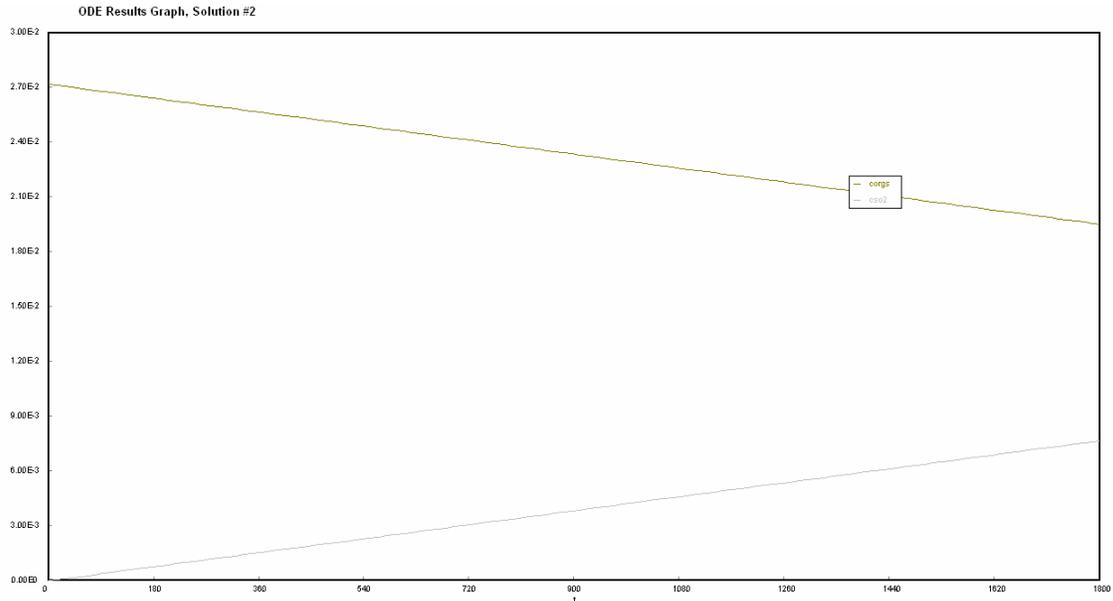


Table 6: Organic Sulfur reaction and SO₂ production

Mass Products per Batch

$$0.0018175 \frac{\text{kmolS}}{\text{m}^3} * \frac{32\text{kgS}}{\text{kmolS}} * 100\text{m}^3 = 5.816\text{kgS}$$

$$0.0004362 \frac{\text{kmolFeS}_2}{\text{m}^3} * \frac{119.85\text{kgFeS}_2}{\text{kmolFeS}_2} * 100\text{m}^3 = 5.228\text{kgFeS}_2$$

$$0.23388 \frac{\text{kmolH}^+}{\text{m}^3} * \frac{1.01\text{kgH}^+}{\text{kmolH}^+} * 100\text{m}^3 = 23.622\text{kgH}^+$$

$$0.23388 \frac{\text{kmolH}_2\text{SO}_4}{\text{m}^3} * \frac{98.02\text{kgH}_2\text{SO}_4}{\text{kmolH}_2\text{SO}_4} * 100\text{m}^3 = 2292.5\text{kgH}_2\text{SO}_4$$

Initial mass of FeS₂:

$$70 \frac{\text{tonscoal}}{\text{hr}} * \frac{907\text{kg}}{\text{tons}} * 0.01825 = 1158.69\text{kgFeS}_2$$

In the United States, most gypsum is used to manufacture wallboard and plaster for homes, offices, and commercial buildings. An average new American home uses approximately 7.31 metric tons (t) of gypsum (Mineral Information Institute, 2001). Worldwide, gypsum is used in portland cement, which is used in concrete for bridges, buildings, highways, and many other structures that are part of our everyday life.

Apparent domestic consumption was more than 36.2×10^6 t in 2004. This was about a 9.3% increase in U.S. gypsum consumption compared with that of 2003. In 2004, the average values reported by U.S. producers were about \$21.10 per ton for calcined gypsum.

Profitability Analysis¹⁹

In order to determine the cost and profitability of our oxydesulfurization plant design, a capital cost and investment estimation was carried out as well as a rigorous profitability analysis. To determine the cost of our equipment, we contacted various companies such as UOP, BP and Jacobs Consultants; we also obtained data from the Perry's Chemical Engineering Handbook. Below is the cost of equipment for the plant, capital investment costs as well as other cost estimations. The formulas for these calculations were taken from 'Product and Process Design Principles' (Seider, Seader & Lewin 2004).

Equipment Cost

Equipment	Quantity	Capital Cost	Installation Factor	Fabrication Cost
Fluid Bed Reactor	1	\$ 1,000,000.00	4.16	\$ 4,160,000.00
Heat Exchanger	2	\$ 60,000.00	3.17	\$ 190,200.00
Compressor	2	\$ 266,000.00	2.15	\$ 571,900.00
Crusher/Grinder	1	\$ 130,000.00	1.39	\$ 180,700.00
Secondary Reactor	1	\$ 12,000.00	3.05	\$ 36,600.00
Turbine	2	\$ 266,000.00	2.15	\$ 571,900.00
Rotary Kiln Air Dryer	1	\$ 459,000.00	2.06	\$ 945,540.00
			Total	\$ 6,656,840.00

Capital Investment Costs

Total bare-module costs for fabricated equipment (Cfe)	\$ 6,656,840.00
Total bare-module costs for spares (Cspare)	\$ 33,284.20
Total bare-module costs for storage and surge tanks (Cstorage)	\$ 29,955.78
Total bare module investment (Ct_{bm})	\$ 6,720,079.98
Cost of site preparation (Csite)	\$ 665,684.00
Cost of Service Facilities (Cserv)	\$ 332,842.00
Allocated cost for utility plants and related facilities (Calloc)	\$ 665,684.00
Total direct permanent investment (Cd_{pi})	\$ 1,664,210.00

¹⁹ "Product & Process Design Principles", Seider, Seader and Lewin (2004)
Perry's Chemical Engineering Handbook

Cost of contingencies and contractor's fee (Ccont)	\$ 249,631.50
Total depreciable capital (Ctdc)	\$ 8,633,921.48
Cost of land (Cland)	\$ 172,678.43
Cost of royalties (Croyal)	\$ 172,678.43
Cost of plant startup (Cstartup)	\$ 863,392.15
Total permanent investment (Ctpi)	\$ 1,208,749.01
Working Capital (Cwc)	\$ 4,504,055.16
Total capital investment (Ctci)	\$ 14,346,725.65

In order to determine the annual sales revenues, production and operating costs, a cost sheet was created to account for the various sectors of the plant on a production basis of 70tons/hour of clean (desulfurized) coal or 554,400tons/year. Also, the plant operating days/year was determined to be 330 days/year.

Cost Sheet

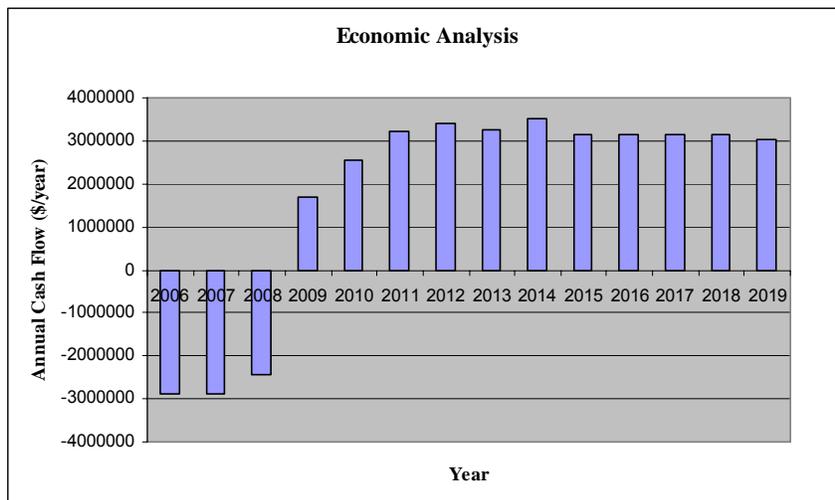
Utilities	Rate Factor	Cost per Year
Steam (1160psig)	\$4.03/ton	\$ 3,010,392.00
Raw Coal	\$29.00/ton	\$16,077,600.00
Water for cooling	\$0.04/ton	\$ 26,196.25
Limestone	\$18.86/ton	\$ 3,969,782.55
Oxygen	\$100.00/ton	\$16,632,000.00
Operations (labor-related)		
Direct Wages and benefits (DW&B)	\$30/operator-hr	\$ 2,376,000.00
Direct Salaries and benefits	15% DW&B	\$ 356,400.00
Operating supplies and services	6% DW&B	\$ 142,560.00
Technical Assistance to manufacturing	52000/yr	\$ 156,000.00
Control Lab	57000/yr	\$ 114,000.00
Maintenance (M)		
Wages and Benefits (MW&B)	4.5% Ctdc	\$ 388,526.47
Salaries and benefits	25% MW&B	\$ 97,131.62
Materials and services	100% MW&B	\$ 388,526.47
Maintenance overhead	5% MW&B	\$ 19,426.32
Maintenance + Overhead (M&O)		\$ 4,038,570.87
Operating Overhead		
General Plant Overhead	7.1% M&O	\$ 286,738.53
Mechanical Dept services	2.4% M&O	\$ 96,925.70
Employee Relations dept	5.9% M&O	\$ 238,275.68
Business Services	7.4% M&O	\$ 298,854.24
Property Taxes and Insurance	2% Ctdc	\$ 172,678.43
Depreciation		
Direct Plant	8% (Ctdc- 1.18Calloc)	\$ 627,873.15
Allocated Plant	6% 1.18 Calloc	\$ 47,130.43
COST OF MANUFACTURE (COM)	Sum of above	\$45,523,017.84

Clean Coal	\$90.58/ton	\$50,217,552.00
Gypsum	\$6.95/ton	\$ 3,852,738.07
Total Sales		\$54,070,290.07
General Expenses		
Selling/transfer expense	3% sales	\$ 1,622,108.70
Administrative expense	2.0% sales	\$ 1,081,405.80
Management incentive	1.25% sales	\$ 675,878.63
TOTAL GENERAL EXPENSES (GE)		\$ 3,379,393.13
TOTAL PRODUCTION COST	COM+GE	\$48,902,410.97
SALES - TOTAL PRODUCTION COST		\$ 5,167,879.10

The Pre-tax or Gross Earnings/year was obtained from the Cost Sheet table above as the difference between the Total Sales and the Total Production Cost which and was \$5,167,879. This indicated a profit of \$4.32/ton of desulfurized coal. However, due to the government and state tax of 37%, the Net Earnings obtained was \$3,255,763/year. The Return on Investment (R.O.I) obtained from this approximate analysis was 23%. The R.O.I was calculated as the ratio between the Net Earnings and the Total Capital Investment (Ctci).

Rigorous Profitability Analysis

The total annual sales revenues, production cost and all of the above profitability conclusions were derived at a given point in time in the life of the plant. This time is assumed to be after 3 years of installation and gradual start-up of the plant, when the plant begins to run at full capacity. In the first year, the plant is assumed to run at only 45% of its capacity, 67.5% in its second year and 90% in the third and subsequent years. Due to the compounding effects of inflation and interest rates, the U.S. Internal Revenue Service requires a profitability analysis to be done over a few years. In this case, the analysis is done over 10 years of the plants life after the 3rd operating year. The following chart shows the profitability/annual cash flow of the plant after accounting for inflation and an annual interest rate of 20%.



Coal Safety Procedures for the Coking Industry

- Volatile chemicals from coal gas emissions, such as aromatic hydrocarbons, carbon monoxide, and ammonia, can be hazardous to worker's health, and may encompass cancer-causing agents.
- Workers must be supplied with proper insulated safety gear, in order to prevent burns and other fatal injuries, from the process of removing the coke from the ovens after processing.
- The company must also be in charge of cleaning the gear on a regular basis, to ensure that the clothing is free of contaminants.
- Sealants for doors and other equipment involved in the industry must be free of asbestos.
- Periodic air monitoring devices must be installed over coke ovens, in order to track the forming pollutants in the air, and warn employees when a harmful dose is present.

Since many of the gases formed from the coking process may be cancerous, early detection cancer screening procedures must be implemented by the company with no cost to the employee²⁰.

²⁰ "Code of practice on Safety and Health in the Iron and Steel Industry," International Labour Organization, Geneva, 2005

Recommendations

Traditionally Chemical Engineering oriented IPROs are not continued beyond one semester. While this trend also seems appropriate for this particular IPRO there is a significant amount of work remaining on this idea. Limiting factors affecting the quality of calculations include reliance on kinetics values garnered from research done by others. The conclusions and rate equations established in these papers are questionable. It was beyond the scope of our IPRO to conduct thermodynamic and reaction kinetics experimental research, there was no alternative to using potentially excessive operating conditions in order to meet reaction requirements set by experimented with different goals than the goals of this IPRO.

If this IPRO were to be continued the most important condition will be generating independent kinetics data. While there likely will not be an extreme cost associated with this, generating heterogeneous catalytic reaction rates is a very time consuming process and generally something that relies on vast experience and not trusted in the hands of undergraduate students.

Acknowledgements

Thank you to our advisor Professor Mohammed Reza Ehsani for guidance throughout the project on which steps to take next. Also thank you to Professor Javad Abbasian for additional guidance and suggestions.

Appendix 1: HYSYS Data Sheets

1		TEAM LND Calgary, Alberta CANADA	Case Name: E:\OXYDESULFURIZATION HYSYS SIM_6B.HSC
2			Unit Set: SI
3			Date/Time: Tue Nov 28 21:00:55 2006
4			
5			

Workbook: Case (Main)

Material Streams

Name	STEAM INLET	AIR INLET	AIR/STEAM TO RE	COAL INLET	COAL TO REACTO
Vapour Fraction	1.0000	0.0000	1.0000	0.1450	0.1450
Temperature (C)	500.0 *	-148.9	260.0 *	25.00 *	260.0 *
Pressure (kPa)	8000 *	8000 *	8000	1000 *	8000 *
Molar Flow (kgmole/h)	1058	595.3	1653	3189	3189
Mass Flow (kg/h)	1.905e+004	1.905e+004 *	3.810e+004	6.350e+004 *	6.350e+004
Liquid Volume Flow (m3/h)	19.09	16.75	35.84	40.50	40.50
Heat Flow (kJ/h)	-2.388e+008	-6.487e+006	-2.453e+008	6.882e+007	9.316e+007
Name	VAPOR REACTOR	LIQUID REACTOR	ADJ REACTOR OU	COAL ADJ OUTLET	REACTOR 2 VAPO
Vapour Fraction	1.0000	0.0000	0.7352	1.0000	1.0000
Temperature (C)	260.0 *	260.0	260.0 *	260.0 *	485.0 *
Pressure (kPa)	8000	8000	7000 *	4400 *	4000
Molar Flow (kgmole/h)	1535	2690	1073	461.9	1049
Mass Flow (kg/h)	4.400e+004	5.761e+004	3.032e+004	1.367e+004	2.562e+004
Liquid Volume Flow (m3/h)	40.89	33.73	26.06	14.83	26.84
Heat Flow (kJ/h)	-2.560e+008	-2.389e+012	-2.675e+008	3.220e+006	-2.668e+008
Name	REACTOR 2 LIQUI	Cooling Water IN	Cooling Water OUT	Flue Gas	Neutralization
Vapour Fraction	0.0000	0.0000	1.0000	1.0000	0.0000
Temperature (C)	485.0	25.00 *	447.5	400.0 *	25.00 *
Pressure (kPa)	4000	7075	7061	6993	101.3 *
Molar Flow (kgmole/h)	199.8	1.280e+008	1.262e+004	1073	41.00
Mass Flow (kg/h)	2.551e+004	2.305e+009	2.274e+005	3.032e+004	4104 *
Liquid Volume Flow (m3/h)	10.44	2.310e+006	227.8	26.06	1.507
Heat Flow (kJ/h)	-2.086e+008	-3.650e+013	-2.876e+009	-2.523e+008	-4.949e+007
Name	Limestone	Cooling Water OUT	To atmosphere	Cooling Water OUT	COOLING 1
Vapour Fraction	0.1112	1.0000	1.0000	0.0000	0.0000
Temperature (C)	400.0 *	472.1	164.5	250.0	250.0 *
Pressure (kPa)	4000 *	7054	101.3 *	7068	7068
Molar Flow (kgmole/h)	224.8	1.262e+004	1049	1.279e+008	1.280e+008
Mass Flow (kg/h)	2.080e+004 *	2.274e+005	2.562e+004	2.305e+009	2.305e+009
Liquid Volume Flow (m3/h)	8.048	227.8	26.84	2.310e+006	2.310e+006
Heat Flow (kJ/h)	-2.095e+008	-2.862e+009	-2.791e+008	-3.411e+013	-3.412e+013
Name	Coal Heat Exit	500 C Steam	Reactor 2 Preheat	Fresh Limestone	Reactor 2 Preheat'
Vapour Fraction	0.0000	1.0000	1.0000	0.1112	1.0000
Temperature (C)	250.0	500.0	500.0	25.00 *	470.0 *
Pressure (kPa)	7061	8000	8000	4000 *	7993
Molar Flow (kgmole/h)	1.279e+008	1.262e+004	1.156e+004	224.8	1.156e+004
Mass Flow (kg/h)	2.305e+009	2.274e+005	2.083e+005	2.080e+004	2.083e+005
Liquid Volume Flow (m3/h)	2.310e+006	227.8	208.7	8.048	208.7
Heat Flow (kJ/h)	-3.411e+013	-2.850e+009	-2.611e+009	-2.412e+008	-2.626e+009
Name	Excess Steam	Clean Coal Stream	Ash & Sulfate Strear	Ash	Sulfate
Vapour Fraction	1.0000	0.0000	0.0000	0.0000	0.0000
Temperature (C)	408.4	181.7	181.7	181.7	181.7
Pressure (kPa)	7986	1200	1200 *	1200	1200
Molar Flow (kgmole/h)	1.156e+004	0.0000	1.279e+008	2.559e+007	1.024e+008
Mass Flow (kg/h)	2.083e+005	0.0000	2.305e+009	4.610e+008	1.844e+009
Liquid Volume Flow (m3/h)	208.7	0.0000	2.310e+006	4.619e+005	1.848e+006
Heat Flow (kJ/h)	-2.658e+009	0.0000	-3.650e+013	-7.778e+012	-2.872e+013

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Workbook: Case (Main) (continued)

Material Streams (continued)

11	Name	Gas	Cooling 1'	Water To Neutraliza	water to neutralizatic	Water Vapor
12	Vapour Fraction	0.9933	0.0000	0.0000	0.0000	0.0000
13	Temperature (C)	188.2	250.0	177.9 *	177.9 *	181.7
14	Pressure (kPa)	1200	7068	7054 *	7054	1200
15	Molar Flow (kgmole/h)	0.0000	1.262e+004	1.279e+008 *	1.279e+008	0.0000
16	Mass Flow (kg/h)	0.0000	2.274e+005	2.305e+009	2.305e+009	0.0000
17	Liquid Volume Flow (m3/h)	0.0000	227.8	2.310e+006	2.310e+006	0.0000
18	Heat Flow (kJ/h)	0.0000	-3.365e+009	-3.494e+013	-3.494e+013	0.0000
19	Name	Steam to Atmospher				
20	Vapour Fraction	1.0000 *				
21	Temperature (C)	99.96				
22	Pressure (kPa)	101.3 *				
23	Molar Flow (kgmole/h)	1.156e+004				
24	Mass Flow (kg/h)	2.083e+005				
25	Liquid Volume Flow (m3/h)	208.7				
26	Heat Flow (kJ/h)	-2.758e+009				

Compositions

29	Name	STEAM INLET	AIR INLET	AIR/STEAM TO RE/	COAL INLET	COAL TO REACTO
30	Comp Mole Frac (Ammonia)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
31	Comp Mole Frac (CO2)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
32	Comp Mole Frac (Oxygen)	0.0000 *	1.0000 *	0.3602	0.0576 *	0.0576
33	Comp Mole Frac (H2O)	1.0000 *	0.0000 *	0.6398	0.0000 *	0.0000
34	Comp Mole Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0874 *	0.0874
35	Comp Mole Frac (SO2)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
36	Comp Mole Frac (Organic Sul*)	0.0000 *	0.0000 *	0.0000	0.1028 *	0.1028
37	Comp Mole Frac (Pyrite*)	0.0000 *	0.0000 *	0.0000	0.0278 *	0.0278
38	Comp Mole Frac (Fe(II)SO4*)	0.0000 *	0.0000 *	0.0000	0.0021 *	0.0021
39	Comp Mole Frac (Argon)	*** *	*** *	***	*** *	***
40	Comp Mole Frac (Fe(III)2O3*)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
41	Comp Mole Frac (H2SO4)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
42	Comp Mole Frac (S_Rhombic)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
43	Comp Mole Frac (Fe(III)SO4*)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
44	Comp Mole Frac (Hydrogen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
45	Comp Mole Frac (Carbon)	0.0000 *	0.0000 *	0.0000	0.7223 *	0.7223
46	Comp Mole Frac (CaCO3*)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
47	Comp Mole Frac (CaSO3*)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
48	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

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TEAM LND
 Calgary, Alberta
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Workbook: Case (Main) (continued)

Compositions (continued)

11	Name	VAPOR REACTOR	LIQUID REACTOR	ADJ REACTOR OU	COAL ADJ OUTLET	REACTOR 2 VAPO
12	Comp Mole Frac (Ammonia)	0.0000	0.0000	0.0000	0.0000	0.0000
13	Comp Mole Frac (CO2)	0.0000	0.0000	0.0000	0.0000	0.1871
14	Comp Mole Frac (Oxygen)	0.1366	0.0001	0.0244	0.3972	0.0020
15	Comp Mole Frac (H2O)	0.5316	0.0746	0.7605	0.0000	0.7779
16	Comp Mole Frac (Nitrogen)	0.1814	0.0000	0.0000	0.6028	0.0000
17	Comp Mole Frac (SO2)	0.1504	0.0016	0.2151	0.0000	0.0330
18	Comp Mole Frac (Organic Sul*)	0.0000	0.0344	0.0000	0.0000	0.0000
19	Comp Mole Frac (Pyrite*)	0.0000	0.0000	0.0000	0.0000	0.0000
20	Comp Mole Frac (Fe(II)SO4*)	0.0000	-0.0000	0.0000	0.0000	0.0000
21	Comp Mole Frac (Argon)	***	***	***	***	***
22	Comp Mole Frac (Fe(III)2O3*)	0.0000	0.0000	0.0000	0.0000	0.0000
23	Comp Mole Frac (H2SO4)	0.0000	0.0152	0.0000	0.0000	0.0000
24	Comp Mole Frac (S_Rhombic)	0.0000	0.0000	0.0000	0.0000	0.0000
25	Comp Mole Frac (Fe(III)SO4*)	0.0000	0.0177	0.0000	0.0000	0.0000
26	Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
27	Comp Mole Frac (Carbon)	0.0000	0.8563	0.0000	0.0000	0.0000
28	Comp Mole Frac (CaCO3*)	0.0000	0.0000	0.0000	0.0000	0.0000
29	Comp Mole Frac (CaSO3*)	0.0000	0.0000	0.0000	0.0000	0.0000
30	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
31	Name	REACTOR 2 LIQUIE	Cooling Water IN	Cooling Water OUT	Flue Gas	Neutralization
32	Comp Mole Frac (Ammonia)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
33	Comp Mole Frac (CO2)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
34	Comp Mole Frac (Oxygen)	0.0000	0.0000 *	0.0000	0.0244	0.0000 *
35	Comp Mole Frac (H2O)	0.0000	1.0000 *	1.0000	0.7605	0.0000 *
36	Comp Mole Frac (Nitrogen)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
37	Comp Mole Frac (SO2)	0.0000	0.0000 *	0.0000	0.2151	0.0000 *
38	Comp Mole Frac (Organic Sul*)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
39	Comp Mole Frac (Pyrite*)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
40	Comp Mole Frac (Fe(II)SO4*)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
41	Comp Mole Frac (Argon)	***	*** *	***	***	*** *
42	Comp Mole Frac (Fe(III)2O3*)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
43	Comp Mole Frac (H2SO4)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
44	Comp Mole Frac (S_Rhombic)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
45	Comp Mole Frac (Fe(III)SO4*)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
46	Comp Mole Frac (Hydrogen)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
47	Comp Mole Frac (Carbon)	0.0000	0.0000 *	0.0000	0.0000	0.0000 *
48	Comp Mole Frac (CaCO3*)	0.0182	0.0000 *	0.0000	0.0000	1.0000 *
49	Comp Mole Frac (CaSO3*)	0.4909	0.0000 *	0.0000	0.0000	0.0000 *
50	Comp Mole Frac (CaSO4*)	0.4909 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

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Workbook: Case (Main) (continued)

Compositions (continued)

11	Name	Limestone	Cooling Water OUT	To atmosphere	Cooling Water OUT	COOLING 1
12	Comp Mole Frac (Ammonia)	0.0000 *	0.0000	0.0000	0.0000	0.0000
13	Comp Mole Frac (CO2)	0.0000 *	0.0000	0.1871	0.0000	0.0000
14	Comp Mole Frac (Oxygen)	0.1112 *	0.0000	0.0020	0.0000	0.0000
15	Comp Mole Frac (H2O)	0.0000 *	1.0000	0.7779	1.0000	1.0000
16	Comp Mole Frac (Nitrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000
17	Comp Mole Frac (SO2)	0.0000 *	0.0000	0.0330	0.0000	0.0000
18	Comp Mole Frac (Organic Sul*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
19	Comp Mole Frac (Pyrite*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
20	Comp Mole Frac (Fe(II)SO4*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
21	Comp Mole Frac (Argon)	*** *	***	***	***	***
22	Comp Mole Frac (Fe(III)2O3*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
23	Comp Mole Frac (H2SO4)	0.0000 *	0.0000	0.0000	0.0000	0.0000
24	Comp Mole Frac (S_Rhombic)	0.0000 *	0.0000	0.0000	0.0000	0.0000
25	Comp Mole Frac (Fe(III)SO4*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
26	Comp Mole Frac (Hydrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000
27	Comp Mole Frac (Carbon)	0.0000 *	0.0000	0.0000	0.0000	0.0000
28	Comp Mole Frac (CaCO3*)	0.8888 *	0.0000	0.0000	0.0000	0.0000
29	Comp Mole Frac (CaSO3*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
30	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
31	Name	Coal Heat Exit	500 C Steam	Reactor 2 Preheat	Fresh Limestone	Reactor 2 Preheat'
32	Comp Mole Frac (Ammonia)	0.0000	0.0000	0.0000	0.0000	0.0000
33	Comp Mole Frac (CO2)	0.0000	0.0000	0.0000	0.0000	0.0000
34	Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.1112	0.0000
35	Comp Mole Frac (H2O)	1.0000	1.0000	1.0000	0.0000	1.0000
36	Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
37	Comp Mole Frac (SO2)	0.0000	0.0000	0.0000	0.0000	0.0000
38	Comp Mole Frac (Organic Sul*)	0.0000	0.0000	0.0000	0.0000	0.0000
39	Comp Mole Frac (Pyrite*)	0.0000	0.0000	0.0000	0.0000	0.0000
40	Comp Mole Frac (Fe(II)SO4*)	0.0000	0.0000	0.0000	0.0000	0.0000
41	Comp Mole Frac (Argon)	***	***	***	***	***
42	Comp Mole Frac (Fe(III)2O3*)	0.0000	0.0000	0.0000	0.0000	0.0000
43	Comp Mole Frac (H2SO4)	0.0000	0.0000	0.0000	0.0000	0.0000
44	Comp Mole Frac (S_Rhombic)	0.0000	0.0000	0.0000	0.0000	0.0000
45	Comp Mole Frac (Fe(III)SO4*)	0.0000	0.0000	0.0000	0.0000	0.0000
46	Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
47	Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000	0.0000	0.0000
48	Comp Mole Frac (CaCO3*)	0.0000	0.0000	0.0000	0.8888	0.0000
49	Comp Mole Frac (CaSO3*)	0.0000	0.0000	0.0000	0.0000	0.0000
50	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

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Workbook: Case (Main) (continued)

Compositions (continued)

11	Name	Excess Steam	Clean Coal Stream	Ash & Sulfate Stream	Ash	Sulfate
12	Comp Mole Frac (Ammonia)	0.0000	0.0000	0.0000	0.0000	0.0000
13	Comp Mole Frac (CO2)	0.0000	0.0002	0.0000	0.0000	0.0000
14	Comp Mole Frac (Oxygen)	0.0000	0.0031	0.0000	0.0000	0.0000
15	Comp Mole Frac (H2O)	1.0000	0.9830	1.0000	0.9999	1.0000
16	Comp Mole Frac (Nitrogen)	0.0000	0.0137	0.0000	0.0000	0.0000
17	Comp Mole Frac (SO2)	0.0000	0.0000	0.0000	0.0000	0.0000
18	Comp Mole Frac (Organic Sul*)	0.0000	0.0000	0.0000	0.0000	0.0000
19	Comp Mole Frac (Pyrite*)	0.0000	0.0000	0.0000	0.0000	0.0000
20	Comp Mole Frac (Fe(II)SO4*)	0.0000	0.0000	0.0000	0.0000	0.0000
21	Comp Mole Frac (Argon)	***	***	***	***	***
22	Comp Mole Frac (Fe(III)2O3*)	0.0000	0.0000	0.0000	0.0000	0.0000
23	Comp Mole Frac (H2SO4)	0.0000	0.0000	0.0000	0.0000	0.0000
24	Comp Mole Frac (S_Rhombic)	0.0000	0.0000	0.0000	0.0000	0.0000
25	Comp Mole Frac (Fe(III)SO4*)	0.0000	0.0000	0.0000	0.0000	0.0000
26	Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
27	Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000	0.0000	0.0000
28	Comp Mole Frac (CaCO3*)	0.0000	0.0000	0.0000	0.0000	0.0000
29	Comp Mole Frac (CaSO3*)	0.0000	0.0000	0.0000	0.0000	0.0000
30	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
31	Name	Gas	Cooling 1'	Water To Neutralizat	water to neutralizatio	Water Vapor
32	Comp Mole Frac (Ammonia)	0.0000	0.0000	0.0000 *	0.0000	0.0000
33	Comp Mole Frac (CO2)	0.0000	0.0000	0.0000 *	0.0000	0.0000
34	Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
35	Comp Mole Frac (H2O)	1.0000	1.0000	1.0000 *	1.0000	1.0000
36	Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
37	Comp Mole Frac (SO2)	0.0000	0.0000	0.0000 *	0.0000	0.0000
38	Comp Mole Frac (Organic Sul*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
39	Comp Mole Frac (Pyrite*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
40	Comp Mole Frac (Fe(II)SO4*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
41	Comp Mole Frac (Argon)	***	***	*** *	***	***
42	Comp Mole Frac (Fe(III)2O3*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
43	Comp Mole Frac (H2SO4)	0.0000	0.0000	0.0000 *	0.0000	0.0000
44	Comp Mole Frac (S_Rhombic)	0.0000	0.0000	0.0000 *	0.0000	0.0000
45	Comp Mole Frac (Fe(III)SO4*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
46	Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
47	Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000 *	0.0000	0.0000
48	Comp Mole Frac (CaCO3*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
49	Comp Mole Frac (CaSO3*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
50	Comp Mole Frac (CaSO4*)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

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Workbook: Case (Main) (continued)

Compositions (continued)

11	Name	Steam to Atmospher			
12	Comp Mole Frac (Ammonia)	0.0000			
13	Comp Mole Frac (CO2)	0.0000			
14	Comp Mole Frac (Oxygen)	0.0000			
15	Comp Mole Frac (H2O)	1.0000			
16	Comp Mole Frac (Nitrogen)	0.0000			
17	Comp Mole Frac (SO2)	0.0000			
18	Comp Mole Frac (Organic Sul*)	0.0000			
19	Comp Mole Frac (Pyrite*)	0.0000			
20	Comp Mole Frac (Fe(II)SO4*)	0.0000			
21	Comp Mole Frac (Argon)	***			
22	Comp Mole Frac (Fe(III)2O3*)	0.0000			
23	Comp Mole Frac (H2SO4)	0.0000			
24	Comp Mole Frac (S_Rhombic)	0.0000			
25	Comp Mole Frac (Fe(III)SO4*)	0.0000			
26	Comp Mole Frac (Hydrogen)	0.0000			
27	Comp Mole Frac (Carbon)	0.0000			
28	Comp Mole Frac (CaCO3*)	0.0000			
29	Comp Mole Frac (CaSO3*)	0.0000			
30	Comp Mole Frac (CaSO4*)	0.0000 *			

Energy Streams

31	Name	Q COAL	REACTOR COOLIN	REACTOR 2 COOLI	Heat	Work 2
32	Heat Flow (kJ/h)	2.435e+007	-2.389e+012	-1.350e+007	1.517e+007	1.230e+007
33	Name	Limestone Preheat	Separator	Heating for Steam	Neutralization Energy	Electricity
34	Heat Flow (kJ/h)	3.166e+007	-8.318e+006	4.893e+008	8.303e+011	1.004e+008

Unit Ops

35	Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
36	MIX-102	Mixer	STEAM INLET AIR INLET	AIR/STEAM TO REACTOR	No	500.0 *
37	SET-3	Set			No	500.0 *
38	X-101	Component Splitter	VAPOR REACTOR EXIT Separator	ADJ REACTOR OUTLET COAL ADJ OUTLET	No	500.0 *
39	TEE-101	Tee	COOLING 1	Cooling Water OUT' Cooling 1'	No	500.0 *
40	TEE-102	Tee	500 C Steam	Reactor 2 Preheat STEAM INLET	No	500.0 *
41	E-101	Heater	COAL INLET Q COAL	COAL TO REACTOR	No	500.0 *
42	E-103	Heater	ADJ REACTOR OUTLET Heat	Flue Gas	No	500.0 *
43	E-108	Heater	Fresh Limestone Limestone Preheat	Limestone	No	500.0 *
44	E-110	Heater	Cooling 1' Heating for Steam	Cooling Water OUT	No	500.0 *
45	CRV-100	Conversion Reactor	AIR/STEAM TO REACTOR COAL TO REACTOR REACTOR COOLING	LIQUID REACTOR EXIT VAPOR REACTOR EXIT REACTOR COOLING	No	500.0 *
46	CRV-101	Conversion Reactor	Flue Gas Limestone REACTOR 2 COOLING	REACTOR 2 LIQUID REACTOR 2 VAPOR REACTOR 2 COOLING	No	500.0 *

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Workbook: Case (Main) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
K-100	Compressor	Cooling Water OUT 2	500 C Steam	No	500.0 *
		Work 2			
K-101	Expander	REACTOR 2 VAPOR	To atmosphere	No	500.0 *
			Work 2		
K-102	Expander	Excess Steam	Steam to Atmosphere	No	500.0 *
			Electricity		
E-106	Cooler	Cooling Water OUT'	Coal Heat Exit	No	500.0 *
			Q COAL		
E-105	Cooler	Reactor 2 Preheat	Reactor 2 Preheat'	No	500.0 *
			Heat		
E-107	Cooler	Reactor 2 Preheat'	Excess Steam	No	500.0 *
			Limestone Preheat		
E-109	Cooler	Coal Heat Exit	water to neutralization'	No	500.0 *
			Neutralization Energy		
E-102	Cooler	Cooling Water IN	COOLING 1	No	500.0 *
			REACTOR COOLING		
E-104	Cooler	Cooling Water OUT	Cooling Water OUT 2	No	500.0 *
			REACTOR 2 COOLING		
V-100	3 Phase Separator	LIQUID REACTOR EXIT	Clean Coal Stream	No	500.0 *
		COAL ADJ OUTLET	Gas		
		Neutralization	Ash & Sulfate Stream		
		Water To Neutralization	Neutralization Energy		
		Neutralization Energy			
RCY-1	Recycle	water to neutralization'	Water To Neutralization	No	3500 *
X-103	Simple Solid Separator	Ash & Sulfate Stream	Ash	No	500.0 *
			Water Vapor		
			Sulfate		

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