Investigating the Production and Use of Transportation Fuels from Indiana Coals

Interim Report for CCTR Advisory Panel Meeting
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Summary

This interim report is in four sections representing the four Purdue research groups that are working on coal to transportation fuels.

Quoting from the planning grant request of March 2006, the objective of the proposal was “the identification and analysis of technological bottlenecks and commercialization barriers associated with the process of converting coal into transportation fuel by (1) improving the design of the process, (2) improving the design of diesel engines and jet turbines which use such fuels, (3) addressing the environmental issues arising from the production and use of such fuels, and (4) addressing the economic and policy issues surrounding the use of such fuels”.

The funding for this project did not become available until early summer 2006, so the progress reported in this interim report represents the accomplishments of the groups from only over the past few months. Three of the four groups however are much further along than might be expected because of two unanticipated developments - Purdue’s hosting of the Lugar Energy Security summit on August 29th, and the state of Indiana’s interest in moving forward, as described in the 2006 Indiana Energy Plan, with a coal to liquids program independent of the outcome of the Obama-Lugar Amendment appropriations process.

Regarding the Energy Security Summit, the Principal Investigator (PI) on the economic/policy issues portion of this proposal, Dr. Wally Tyner, was asked to present a broader policy piece at the Summit dealing with policy alternatives to stimulate private sector investment in all domestic alternative fuels, including both biofuels and fuels derived from coal. This additional responsibility moved forward the time schedule of Dr. Tyner’s work for the CCTR, and the work sponsored by the CCTR has become an integral part of Dr. Tyner’s presentation at the summit.

Regarding the state’s expressed interest in speeding the commercialization of Indiana’s homegrown fuel substitutes as described in the State Energy Plan, the Fischer-Tropsch (FT) production and use groups, have put together a major multi-year, multi PI, multi disciplinary proposal to the state to investigate the production and use of transportation fuels from Indiana coals. This preparation of a follow-on proposal has also moved forward in time the work schedule of the twelve Purdue engineers and scientists involved, which accelerated the progress in the two sections (production and use) of this progress interim report dealing with their accomplishments.

(1) Economic Group

ECONOMIC ANALYSIS OF COAL LIQUIDS POLICY OPTIONS

Wallace E. Tyner, Dileep Birur

Our economic analysis is based on coal to liquids plant cost information contained in the Southern States Energy Board report, *American Energy Security: Building a Bridge to Energy Independence and to a Sustainable Energy Future*, released in July 2006. We used case number five, a 60,000 barrel per day plant with sequestration of CO_2. The total capital cost of the plant is $3.9 billion. Following the case authors, we assumed one third equity and two-thirds debt financing. The debt interest rate is 8 percent and the required minimum return on equity is 15 percent. The assumed inflation rate was 3 percent. We used other economic assumptions provided by the study authors (Table 1). We calculated a break-even price of $43/bbl. crude oil equivalent, close to the $44 obtained by the authors.

Table 1: Economic Assumptions for the Coal Liquids Policy Analysis

Economic Parameter / Assumption		**Value**
Construction Period		3 years
Year 1Incurred Capital Cost Construction		20%
Year 2 Incurred Capital Cost Construction		50%
Year 3 Incurred Capital Cost Construction		30%
1st Year Availability		45%
2nd Year Availability		81%
3rd Year and Beyond Availability		90%
Plant Lifetime	years	25 years
Return on Equity		15%
Depreciation Method		DDB-16 yrs.
Debt:Equity Ratio		2/1
Interest Rate		8%
Inflation Rate		3%
Tax Rate		36%
Electricity Selling Price	$ / MWhr	$35.60
Sulfur Price	$ per ton	$80
Bituminous Coal Price	$ per ton	$36
Subbituminous Coal Price	$ per ton	$11
Lignite Price	$ per ton	$10
Woody Biomass Price	$ per ton dry	$20
Naphtha Value	times diesel value	$0.714

We then introduced stochastics into the analysis, thus far in the form of capital cost uncertainty and oil price uncertainty. Capital cost uncertainty was modeled as a simple triangular distribution. However, oil price was much more complex. We calculated the mean and standard deviation of real annual oil price change over the past 25 years. Twenty five years was chosen because the prices changes were much lower in earlier years. The mean price change was very close to zero, and the standard deviation was $9.20 per year. We constrained annual price changes to plus or minus $23 per year, the largest experienced in the past 25 years. Future price scenarios were then simulated with a constraint that the future price could not fall below $15 (2006$), the lowest price in the past 25 years nor higher than $200, chosen arbitrarily.[1] Under these conditions, we simulated a series of future prices with base prices ranging from $40 to $70. All of this uncertainty was captured in a Monte Carlo simulation using @Risk software and doing 10,000 iterations for each simulation.

Outputs included net present value of the project, internal rate of return, chance of a loss, and present value and annualized value of the sum of diesel and naptha sales. For each of these outputs, we have the mean (expected value), standard deviation, and all elements of the probability distribution.

The simulations to date have been done for the base case and the policy of a variable subsidy. We tested different levels of the variable subsidy with it kicking in at $35, $40, and $45. That is, there is no subsidy if crude oil average annual price is above the stipulated level, but a variable subsidy equal to the difference between the market price and the stipulated level if the market price is below the subsidy floor. For example, if market price was $40 and the price floor $45, there would be a subsidy of $5 per barrel of crude oil equivalent fuel produced. If the market price is above $45, there is no subsidy. The actual subsidies were converted to diesel using a historic regression relation between crude oil prices and diesel prices.

The key output values are chance of a loss for each price and policy simulation and government cost for each policy alternative. Figure 1 illustrates the probability of a loss for each base price case and for the $45 price floor policy alternative. The interpretation of the graph is as follows. The first number in the number pairs is the base price, and the second is the price floor. For this graph, the price floor is always $45. One can see that if the base price is $40, the chance of a loss with no policy intervention is greater than 50 percent. If the base price is $70, then the probability of a loss is around 10 percent. One can think of the base prices as the central tendency, that is the price around which future prices are expected to move. Just barely visible along the X axis, one can see that the chance of a loss with a $45 price floor subsidy is always zero, regardless of the base price. So clearly, a $45 price floor policy is quite effective at reducing risk and thereby stimulating investment in coal liquids.

Another question is how much would this subsidy cost the government. The answer, of course, depends on what future crude oil prices do. Figure 2 displays the expected government cost for each of the base prices. These costs are expressed in terms of $/gal. of diesel produced. They were calculated as the difference between the diesel sales revenue with and without the policy in effect. The expected costs range from 11 cents per gallon with a $70 base price to 40 cents per gallon with a $40 base price. Any

[1] The results were not very sensitive to the level of this upper limit.

of these costs are less than most estimates of the national security cost of imported oil. Also, of course, if the crude oil price were to remain above $45 for the 25 year life of the plant, the government cost would be zero.

In the future with additional funding, we intend to apply this general approach described to other policy options and to examine other ways of incorporating future price uncertainty. We will also add uncertainty in other variables such as coal cost.

Figure 1

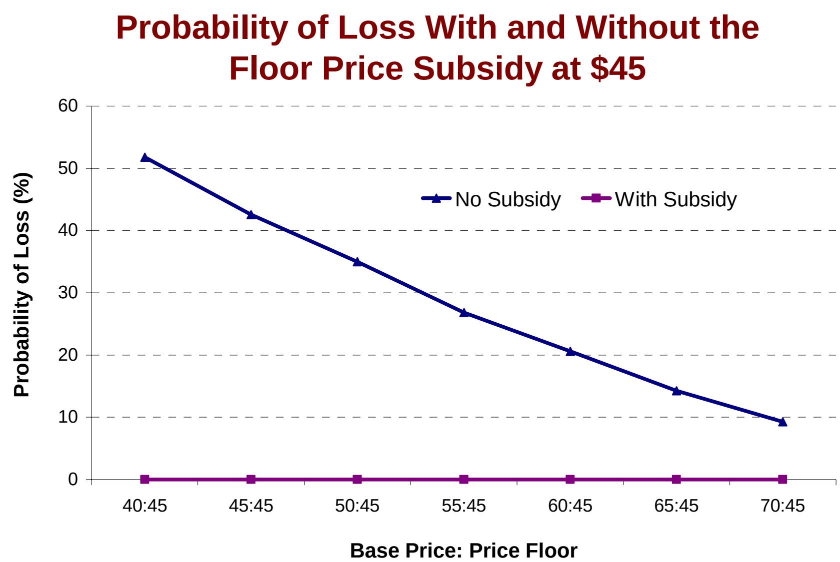
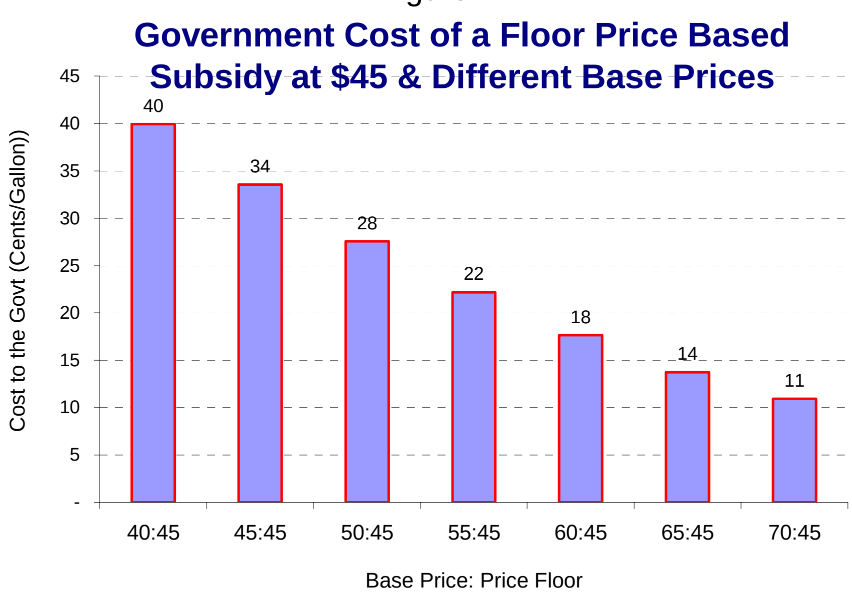


Figure 2



(2) Production Group

Progress Report to be submitted to CCTR August 31, 2006

Rakesh Agrawal, W. Nicholas Delgass
Fabio H. Ribeiro, Navneet Singh

Easy availability, relatively lower cost and high volumetric energy density of liquid fuels were primary reasons for their preferred usage as source of energy for transportation. However, due to the sharp increase in prices of crude oil and speculations that world oil production may reach a peak within the next 10 to 50 years, researchers have started looking at alternate sources of producing liquid fuels. Coal to Liquid (CTL) comes at the forefront of such alternate processes to produce liquid fuels. Since the US and Indiana have large reserves of coal, this coal can be converted to liquid fuels which will help reduce the dependence on imported oil. However, conversion of coal to liquid fuels is laden with a number of technical challenges.

Conversion of coal to liquid fuels can be broken down into two processes: gasification of coal, followed by the production of liquid fuels by the Fischer-Tropsch (FT) process. Diesel produced from FT has a number of attractive properties compared to traditional crude oil derived diesel. Sulfur as well as aromatics are nearly absent in FT diesel. This is because of the fact that it is easy to remove sulfur from high pressure gas streams and the aromatics content is low because of the characteristic FT polymerization process. The FT products are straight chain molecules having very high cetane number so diesel range components are favored. High olefin selectivity is also preferred because olefins can either be used as base chemicals or can easily be upgraded to components with higher octane numbers such as gasoline. Thus, the desired components are diesel range linear components and olefins preferably in the gasoline range. We are trying to find an operating regime to optimize for selectivity without having to worry as much as usual about rate of reaction so that there is no need to go for very high per pass conversion in the FT reactor, consequently we do not necessarily have to focus on having a very highly active catalyst.

In a traditional refinery, about 10% of total energy in crude is lost during processing of crude oil to get a variety of products. However, the energy content of coal used to supply about 13.9 million bbl/d of oil (which is the current consumption rate of transportation sector in US) will be greater than the energy content of 23 million bbl of oil. This is because of process inefficiencies involved in coal to liquid conversion. Large inefficiency in the CTL processes comes from conversion of coal to carbon dioxide in the coal gasifier and in the Fischer-Tropsch (FT) reactor. Due to this reason, twice the amount of carbon dioxide is generated for each gallon of CTL fuels utilization as compared to fuel form petroleum. Generally this carbon dioxide is emitted to the atmosphere. An alternative to produce liquid fuels which will minimize the release of carbon dioxide is thus, a priority. Hence, there is need to increase the energy efficiency of the overall process as well as selectivity to the final liquid fuel. This improvement will decrease the associated emission of carbon dioxide. The current goal of this research is to achieve this improvement at both fronts. A systems analysis is being done to increase the overall efficiency of the process as well as search for a better catalyst is envisioned to increase overall selectivity to the desired fuel. Early results with systems analysis have provided some intriguing insights that are currently under exploration. When substantiated, they have a potential to make a wide impact on energy production and consumption.

We are trying to identify the basic causes of the inefficiency of the over-all CTL process and then, find remedies for the underlying inefficiencies. Since the whole process of conversion of coal gasification to syngas and subsequent CO hydrogenation to liquid fuels is complex, we are using ASPEN to evaluate the effect of this integration. There are a number of parameters like temperature, pressure, catalyst, promoters, H_2/CO ratio and others which affect the product distribution in the FT reactor, which is turn provides the amount of liquid fuel obtained. The ASPEN model of the entire system will enable us to get better insight of the factors which affect the product distribution of the process and how to improve the quantity of liquid fuels. New ideas can be tested considering the entire process from raw coal to the final refined product. This is necessary because the various processes in a plant interact with each other and the overall efficiency cannot be calculated unless the entire process is simulated. We will carry out experiments to verify the insights gained from ASPEN models. The economic feasibility of these CTL processes has not been shown commercially till date and the viability of these processes is largely dependent on the price of crude oil. We are planning to use ASPEN Icarus to study the economics as a function of different parameters.

(3) User Group

Use of Fischer-Tropsch (F/T) Fuels in Gas Turbines and Diesel Engines

John Abraham, Bill Anderson, Jim Carruthers
Steve Heister, Jay Gore, Robert Lucht, Yuan Zheng

The scoping grant from the CCTR to determine issues associated with the use of Fischer-Tropsch (F/T) fuels in diesel engines and gas turbines. The literature on F/T fuels was reviewed and a proposal for the continuation of F/T fuel research was developed. Plans were developed for pursuing research in the areas of combustion of F/T fuel in diesel engines and in developing after treatment technology suited to F/T fuels. A gas turbine combustion facility for testing F/T fuels and measuring emissions has been developed with funding from the State of Indiana 21st Century program. In collaboration with Rolls Royce, an experimental facility for testing the thermal stability of jet fuels, including F/T fuels, has been developed. The potential for future collaborative efforts with Rolls Royce Indiana in the testing and evaluation of F/T fuels for aircraft propulsion has been explored.

Coal to liquid (CTL) fuels can provide a secure and environmentally friendly energy resource for US trucks and for commercial and military aircraft. Recoverable coal in US has the energy content comparable to all of the world's known oil reserves and CTL fuels derived from the F/T process are virtually free of aromatics and sulfur. Combustion of F/T jet fuel therefore produces much less particulate matter (PM) compared to conventional petroleum-derived jet fuels, such as Jet A (commercial) and JP-8 (military), and no SO_X . F/T fuels are also of great interest to US Air Force for the development of paraffinic endothermic jet fuels. Comprehensive knowledge of F/T jet fuel combustion is one of the enabling components for the commercialization of CTL transportation fuels but fundamental combustion data is lacking.

The major emissions from aircraft engines are particulate matter (PM), NOx, CO and unburned hydrocarbons (HC). Most airborne PM consists of particles smaller than 2.5 m in diameter (PM2.5). Soot is formed in the rich regions of nonpremixed combustion and the amount of PM emitted from a combustion system depends on the competition between soot formation and soot oxidation. The molecular structure of the fuel is a very important factor in determining the level of PM emissions. The combustion of aromatics fuels, especially poly-aromatics, is much more likely to produce soot than paraffin combustion. The smoke point is the measure of a fuel's sooting propensity. Conventional jet fuels contain approximately 20% aromatics and usually have a smoke point around 20 mm. Neat F/T fuels typically contain only n-paraffins and iso-paraffins and usually have smoke points above 43 mm. Since the utilization of neat F/T fuels in current engines is complicated by problems with lubricity and compatibility with elastomers and seals, blends of F/T and conventional jet fuels or F/T fuels containing synthetic aromatics have been used commercially in South Africa. These approaches, of course, dilute some benefits of F/T fuels. Gas turbine engine design is another very important factor in determining PM emission. PM emission becomes more severe with increasing operating pressure due to shorter spray penetration and accelerated chemical reaction at higher pressures.

The swirler-stabilized turbulent flames facility and simultaneous stereo PIV and PLIF measurement facility at the Turbulent Combustion Lab and the gas turbine combustor facility at the High Pressure Lab (part of the Rolls-Royce Center of Excellence) provide unique capabilities for the proposed research. At the High Pressure Lab, the recently modernized air system can provide dry air at 950 $^{\circ}$F and 700 psi at flow rates up to 9 lbm/s. The well-instrumented gas turbine combustor facility with an air-cooled liner is designed in a modular fashion to facilitate rapid hardware changes. In addition, the recently installed advanced FT-IR MultiGas Analyzer provides the capability of monitoring a large number of infrared-active species (CO, CO_2, H_2O, NO, NO_2, etc.). Instrumentation to measure total HC and O_2 is also available.

The proposed project will significantly enhance our understanding on key combustion and emission issues in the development of advanced aircraft engines using CTL F/T fuels. The proposed project will also promote the development of diagnostic technologies suitable to investigate combustion and emission in aircraft engines. The knowledge obtained in the proposed project will strongly facilitate the utilization of CTL F/T jet fuels in civilian and military aircraft.

We have also studied many issues associated with combustion of F/T fuel in diesel engines. An attractive feature of F/T diesel fuels is that the production process of the fuel may be modified to change its properties. For example, the cetane number of the fuel may be changed to achieve slower ignition. This may allow better premixing prior to the start of combustion and make it possible to inject the fuel earlier in the compression cycle, thereby approaching premixed combustion. This, in turn may result in lower particulate emissions and either lower or higher NO_x emissions based on the degree of premixing achieved. Similarly, changes in the volatility and lubricity of the fuel can be effected by changing the production process. Increasing the aromatic composition of the fuel may enhance lubricity, but may result in greater PM emissions. Hence, the changes are likely associated with costs and benefits. Careful evaluation is needed to optimize the fuel, the combustion system and the level of aftertreatment required.

As part of the scoping grant diesel combustor facilities and emissions analysis equipment was identified that can be used for future FT fuels research. F/T diesel fuel obtained from Syntroleum, F/T diesel fuel mixed in different proportions with diesel fuel #2, low-sulfur diesel fuel, and with bio-diesels, will be evaluated.

In addition, a comprehensive plan for the development of an after treatment system suitable for diesel engines operating on FT fuels was formulated. The most promising technology for the reduction of NO_x compounds in diesel emissions is the use of NO_x storage and reduction (NSR) catalysts. To take advantage of the lean (i.e. excess oxygen) operation of a diesel engine, the NSR catalyst is operated in a cyclic manner. While the engine is running lean, the catalyst adsorbs NO_x onto an alkaline earth or alkali metal component, i.e. barium or potassium, while the NO is converted to NO_2 on a noble metal that is typically platinum. When the catalyst has been partially saturated, the engine is switched over to rich (i.e. excess fuel) operation for a short period of time. In this rich part of the cycle, the stored NO_x is converted to nitrogen and water which are released to the environment and the storage capacity of the catalyst is regenerated, allowing the cycle to repeat. Because of the large number of potential operating parameters in the engine duty cycle, mathematical models are needed to aid in the understanding of the NSR catalytic system. Our group has developed the first chemically reasonable yet practically workable mathematical models to describe the performance of the NSR catalytic process using simulated diesel exhausts.

(4) Environmental Group

Investigation of the Environmental Implications of Coal to FT Fuel Production

T.P. Seager, L.S. Lee, D. Mu

Introduction

This research is motivated by the hypothesis that understanding the life-cycle environmental implications of transitioning from petroleum-based to coal-based transportation fuels will facilitate creation of technological linkages between the coal processing, gasification and FT fuel production industries with other industries such as construction materials and chemicals. Fostering these linkages is expected to help overcome the principal obstacles to FT fuel investment: economic risks and environmental objections. The economic risks result from the relatively high capital expenditures required of coal-to-liquid-fuels (CTL) production facilities, whereas environmental objections result from the production of waste ash, water or other streams at the production site – even as FT fuels are recognized as burning cleaner in automobile engines. The approach taken in this research is to identify the waste streams typical of FT fuel production and match those with raw material feedstock requirements in other industries that can be co-located with FT fuel production, such as cement or drywall manufacture. Finally, a research agenda for developing the technological processes necessary to couple two or more mutualistic industries shall be proposed.

Progress to date

A draft process flow schematic of the FT fuel production process has been completed (see attached). The primary material and energetic input and output streams have been identified, and are summarized the table below. A number of useful co-products from FT fuel production have already been identified and are employed in the chemicals, plastics or other industries (such as fertilizer).

Input and Output for Coal to Liqiud Fuel Process

INPUT	OUTPUT				
	main product	co-product		by-product	
		material	potential user	material	place for disposal
coal	diesel	liquid N_2	ammonia production	waste N_2	atmosphere
air	LPG	Kr/Xe	lamp production and lab agents	coal fines	mine
primary water		phenol	plastic, medical production	ash from gasifier	landfill
electricity		cresylic acid	chemical production	dust	landfill
		naphtha	chemical Industries	air from steam generation	atmosphere
		sulfur	sulphuric acid production	CO_2	atmosphere
				wastewater	incinerator

However, there are still large volumes of waste material created as by-products of FT fuel production that represent economic and environmental liabilities, including: nitrogen gas, coal ash and fines, waste water (and sludge), and waste heat. Coupling these material streams with the raw material needs of other industries has the potential to reduce both economic costs and environmental effects – thereby speeding adoption of FT fuel technologies.

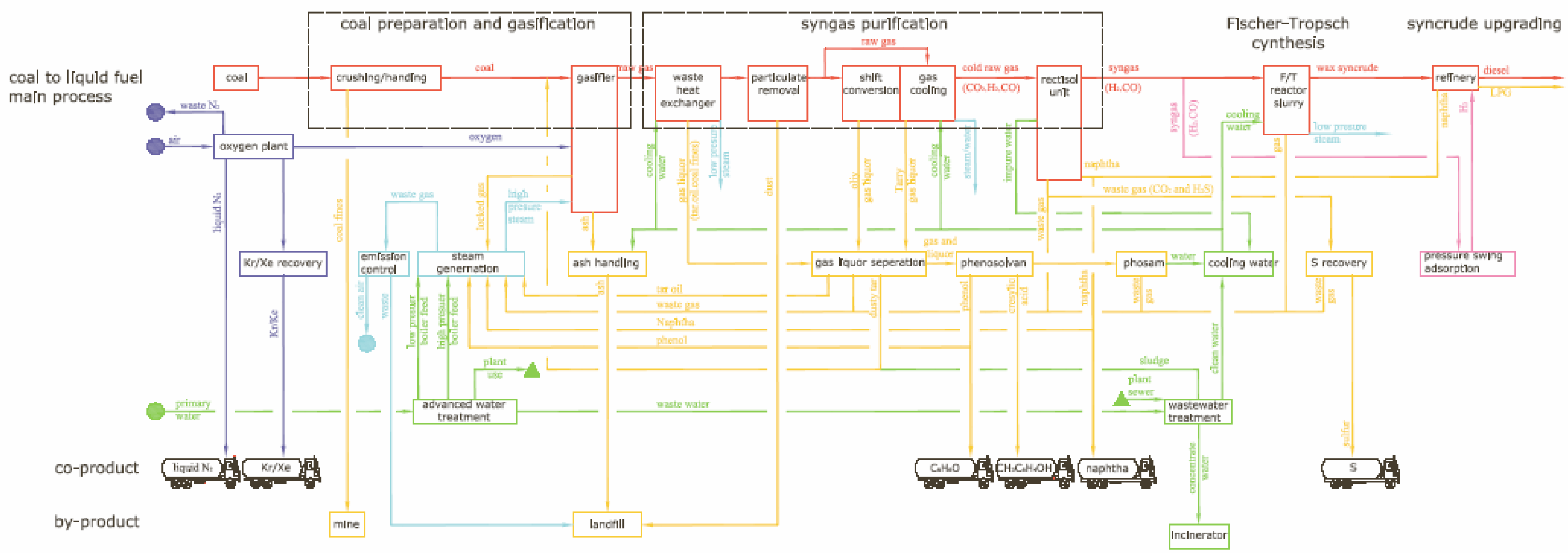
For example, coal ash has successfully been used as a replacement for limestone and other mineral feedstocks in cement production. However, to date only class C coal fly ash (which contains high concentrations of calcium) has been effectively utilized. Consequently, this project has focused on beneficial reuse alternatives for class F fly ash, which is a by-product of current coal combustion technologies. To date, a literature review has identified geopolymer cements as a promising beneficial reuse technology. Geopolymer cements obtain strength from alumino-silicate bonding in the absence of calcium. Unlike ordinary Portland cement, geoploymer cements do not require evolution of carbon dioxide from limestone feedstocks or water to hydrate. Current estimates indicate that the greenhouse gas emissions of geopolymer cements are several times lower than those associated with ordinary cement. Strength and durability characteristics are viewed as favorable. However, the environmental leaching characteristics of geopolymers are untested. If significant concentrations of metals or other environmentally significant chemicals are liberated during use or disposal of geopolymer cements, environmental concerns could present an obstacle to beneficial reuse of FT residues in construction applications.

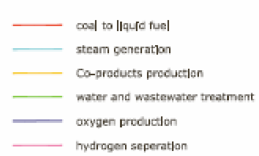
Future Plans

The FT process flow diagram will be further detailed. Our present state of understanding is qualitative. Further investigation is required to develop quantitative or semi-quantitative models. Also, the process diagram will be extended to include use of diesel fuel (the primary product) in the transportation sector by coupling the existing model with the life-cycle emissions data available in the GREET model (developed at Argonne National Labs to model alternative fuel technologies). The result is expected to be an integrated, life-cycle model depicting the material and energy flows and balances that can be expected to represent FT fuel production from mining all the way to dissipation of exhaust gases in the atmosphere. Ultimately, this model will facilitate environmental assessment of hypothetical technological linkages between FT fuel production and other industries.

In addition, this research program will leverage Coal Center resources with teaching assistantships, SURF program resources or other Center for Environment funds to identify and develop the technological linkages necessary to link FT fuel production to mutualistic industries. The initial focus of this work is the production of geopolymer cements from ash – however, other by-product material and energy opportunities are expected to be revealed. With regard to geopolymers, production of geoploymers from both pure and ash materials will be undertaken during the next six months. As geopolymer samples are produced, these will be tested for both strength (i.e., suitability for construction applications) and environmental leaching properties. Ultimately, this is expected to lead to a large-scale structural and environmental testing of structures (such as reinforced concrete beams) made from class F coal fly ash.

The overarching vision of this research program is to create a model for environmental assessment of FT production technologies and identification of further research opportunities that would be attractive to funding agencies such as USDOE, NSF and/or USDA that represent potential partner organizations for the Coal Fuels Alliance and Clean Coal Tech Center.





Flow Diagram of Coal to Liquid Fuel Process

Input and Output for Coal to Liqiud Fuel Process

INPUT	OUTPUT				
	main product	co-product		by-product	
		material	potential user	material	place for disposal
coal	diesel	liquid N_2	ammonia production	waste N_2	atmosphere
air	LPG	Kr/Xe	lamp production and lab agents	coal fines	mine
primary water		phenol	plastic, medical production	ash from gasifier	landfill
electricity		cresylic acid	chemical production	dust	landfill
		naphtha	chemical industries	air from steam generation	atmosphere
		sulfur	sulphuric acid production	CO_2	atmosphere
				wastewater	incinerator