

# **Flash Pyrolysis of Coal in Methane**

**Group:** So-Called Engineers

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## Executive Summary

Flash pyrolysis of coal in an atmosphere of methane is an alternative use of coal to produce high value products that can be used for various petrochemical processes. The process involves taking run of mine (ROM) coal and flash pyrolyzing it at a temperature of 1832 °F and a pressure of 500 psia to produce benzene, toluene, and xylene (BTX), and a fuel gas stream composed of methane, carbon dioxide and carbon monoxide. A “raffinate” stream comprising of approximately 91% heptane and 9% hexane is produced. Additionally, a solid char, with a heating value of 11091 Btu/lb, is produced that is used to heat the reactor during the process.

The process is executed by processing ROM coal to be used in a pyrolysis reactor. The reactor effluent is quenched with a water stream. The resulting stream is cooled in an array of parallel heat exchangers and fed to a flash separator to remove the water from the stream. The product stream is turboexpanded to allow the BTX, heptane and hexane to condense. The majority of the fuel gas stream is separated in the second flash unit where it is purged and then recycled into the reactor after being replenished with a make-up stream. The purge stream is used to heat any remaining parts of the process that aren't heated by the solid char. The product stream is run through a series of distillation and extraction columns to achieve an essentially pure product stream of BTX and a “raffinate” stream. The extraction column involves using a tetraethylene glycol solvent that strips the aromatics (BTX) from the alkanes (heptane and hexane). The tetraethylene glycol is separated and recycled into the extractor.

An economic analysis was completed to evaluate the viability of the base case. To operate the process, \$16.9 million dollars of coal and \$3.8 million dollars of natural gas are required every year. The main products are fuel gas, which can be sold for \$147 million per year and BTX which makes \$81 million per year. The net present value for the process after 20 years with a discount factor of 12% is approximately \$674.62 million dollars with a payback period of 6.25 years. The discounted cash flow analysis yielded an internal rate of return of 22.88% for the base case which exceeds the minimum acceptable rate of return that was set at 12%. Sensitivity analysis determined the total capital investment and the sale price of fuel gas to be the most significant factors in the plant profitability but changing each of these parameters by  $\pm 25\%$  did not lower the IRR below the MARR.

The design for the project currently lends itself to continuing to move forward with the flash pyrolysis plant upon further research into alternative separation processes that would improve product purity and operational efficiency. Once the cash flow stabilizes for the base case, the plant will bring in about \$209.2 million dollars per year and shows the potential for a highly profitable plant.

After extensive study of the base case for this process, future work is planned to improve the process to yield higher purity products as well as to minimize operational inefficiencies. Additionally, because of a 22.88% IRR, it is recommended that the project proceed forward.

## Scope of Work

The scope of this project is to find an alternative method of converting coal into profitable chemical precursors. The alternative method being investigated is the flash pyrolysis of coal in an atmosphere of methane. This design was originally researched in 1986 by Dr. Steinberg at Brookhaven National Laboratory, but the process was never utilized in industry. This may be due, in part, to the high price of methane when this research was first conducted, in addition to the low product yields. Similar experiments in flash pyrolysis use atmospheres of hydrogen or argon gas; however, natural gas is much more affordable and easier to access today. The design problem faced is designing a plant that uses flash pyrolysis of coal in an atmosphere of methane to produce sellable products. Additional challenges include making these products relatively pure for sale and optimizing the process to create the largest profit achievable over the plant's lifetime to create an economically viable process.

## Introduction

Coal serves as a great starting point for numerous products because it can be converted into energy, chemical products, or carbon materials. Pyrolysis is the thermal decomposition of organic materials in the absence of an oxidizing agent. The process of pyrolyzing coal produces numerous carbon materials such as chars, tars, and product liquids and gases. Some organics used commonly for pyrolysis reactions are biomass (wood, agricultural waste, manure) and fossil fuels (coal). A regular pyrolysis reaction typically operates in an inert atmosphere within a certain range of reactor residence times. Pyrolysis reactions can take place over a wide range of temperatures and pressures as well, with the residence time, pressure, and temperature all influencing the distribution of products after the coal has been fed through the reactor. As coal enters a pyrolyzer, two phases of reactions are observable. The first consists of both thermal degradation and cracking of the coal to form light oils, heavy tars, char, and gases. The second phase is a continuation of cracking, evaporation, and repolymerization processes which can alter the final product distribution at longer residence times (Radenovic 2005). A conventional pyrolysis process operates at temperatures ranging from 400-500°C and with residence times ranging from 5-30 minutes. Fast pyrolysis takes place at temperatures of 400-650°C with a residence time of 0.5-2 seconds. The flash pyrolysis process takes place at temperatures ranging from 700-1000°C and has short residence times of less than 0.5 seconds (Steinberg 1986).

The approach used to design this process was a flash pyrolysis of coal in an atmosphere of methane. The justification for using a flash pyrolysis is that at high temperatures and very short residence times, the product distribution shifts to allow for more high value product production (BTX and ethylene). A methane atmosphere was selected for the process due to information taken from Dr. Steinberg's work at Brookhaven National Laboratory that illustrated that an atmosphere of methane provided higher product yields of benzene, toluene, and xylene as well as ethylene. For a flash pyrolysis of coal in an atmosphere of methane, roughly 79% of the dry coal

entering the reactor is converted into char. Approximately 6% of the dry coal is converted to the high value products, benzene, toluene, and xylene (BTX), and approximately 8% of the dry coal is converted to ethylene, another high value product.

The process selected for this project was a flash pyrolysis of coal in an atmosphere of methane, but there are a variety of alternative processes that have been considered or utilized as well. One alternative that is in practice today as research continues to delve deeper into the potential that it has is the use of biomass as the organic fuel source. This process is used to convert the biomass to biofuel that could potentially serve as an alternative to fuel oil or be used to produce gasoline and diesel fuels. The issue with this method is that many of the products that are yielded from biomass pyrolysis are either in too small of quantity to be a viable salable product, or do not have a market demand for the product in order to sustain the pyrolysis plant. Another alternative that was explored in depth before eventually being discarded was a system of refrigerated distillation columns used to separate the high quantities of methane gas from the desired products for the reaction. This alternative required nearly \$80 million dollars per year in refrigeration operational costs alone. As the alternative was investigated further, it became clear that the high operating costs for the plant completely negated all revenue that the desired products produced and made the alternative infeasible due to the complete lack of economic viability. Other separation processes were considered once the refrigerated distillation system was deemed impractical and one potential alternative was an oil absorption tower to separate the larger hydrocarbons from the desired products. This alternative presented some challenges mainly with modeling the system within Aspen+ and with the sizing of equipment for the process. This alternative was also going to be more expensive than the base case which utilized a turbo expander for the separation process. A final alternative that needs to undergo economic analysis is the separation of the benzene, toluene, and xylene mixed stream into three constituent streams. This separation would require more capital upfront and would likely increase utilities by some amount, but it would also allow for higher purity products that would fetch a premium sale price. The economic analysis of this alternative would determine if the profits from the premium sale price outweigh the utility increase.

## **Description of Base Case**

The chemical process designed for the flash pyrolysis of coal in an atmosphere of methane is composed of several unit operations. The process begins with the grinding of ROM coal to provide a more functional and uniform reactant. This coal is then dried in a drying unit in order to reduce the amount of water that is present in the reactor. Once the coal has been dried, the dry coal is fed to the three-stage lock hopper. This allows the coal to be pressurized from atmospheric pressure to the pressure of the pyrolysis reactor and then fed into the reactor safely. Very low residence times are used in the reactor to maximize the rate of heating of the reactants. This provides greater product yields and decreases the production of undesirable products. The products of the reactor are immediately quenched with a stream of liquid water to cool the reaction down to a temperature at which pyrolysis is no longer occurring. This cooled product

stream is then fed to a plate and frame separator in order to remove the char from the reactor effluent. The remaining stream is then condensed in an array of parallel heat exchangers to condense most of the water in the stream. Once cooled, the stream is then separated with the use of a flash separator. The liquid stream out of the flash unit consists almost entirely of water, with some impurities. This water stream will be treated downstream in order to purify the water for further use. The gaseous stream from the flash separator is fed to the turboexpander. The turboexpander allows the heavier components to condense by depressurizing the stream. Additionally, usable work is being produced by expanding the gas which can be used to minimize the amount of electricity that needs to be purchased. This stream is fed into a flash unit where the BTX is separated from a majority of the Fuel Gas (FG). Both streams exit the flash unit and are reheated using a heat exchanger. The FG stream which contains methane, carbon monoxide and carbon dioxide is considered to be a finished product after this separation and will be recycled into the reactor. The recycle stream will have a purge stream to increase the methane concentration in the stream. The purge stream will be diverted to be burned to produce required heating for the process. Additionally, a makeup stream will replenish the methane stream with natural gas. The remaining liquid stream will be sent a distillation column to separate the remainder of the FG from the BTX stream. The FG stream will again be used for any heating requirements around the plant. The BTX stream will then be re-pressurized using a pump. From there the stream will be sent into an extractor to separate hexane and heptane from BTX using tetraethylene glycol as a solvent in liquid-liquid extraction. Two liquid streams will come out of the extractor. The first will be a mixed stream of heptane and hexane and a small amount of the solvent. The stream will be sent to a distillation column and the heptane and hexane will be separated from the solvent and will be sold as “raffinate.” The solvent will be recycled into the extractor. The other stream out of the extractor will contain a solvent rich BTX stream. The stream will be sent into a distillation column that will separate the tetraethylene glycol from the BTX. The BTX stream will be essentially pure and can be sold. The tetraethylene glycol stream will be mixed and recycled and added with a makeup stream to be refed into the extractor.

Before the coal can enter the reactor, ROM coal is processed to achieve the best possible yields. This involves grinding it down into smaller pieces and removing as much of the moisture content as possible. Grinding it down into smaller pieces increases the surface area that is available for reaction. Having more surface area increases the yields of the reaction. Additionally, removing the moisture from the ground coal decreases the possibility of undesirable secondary reactions in the reactor. Additionally, the coal is fed into the reactor using a three-stage lock hopper. The lock hopper allows the coal at atmospheric pressure to be safely transferred into the reactor. The coal enters the first stage which is at atmospheric pressure. The coal is then gravity fed into the second stage where it is purged with inert gas and is slowly increased to the pressure present in the reactor. The coal is then fed into the third stage where it can be continuously fed into the reactor. The second stage is then depressurized back to atmospheric pressure. Dry coal, DRYCOAL Table 1, is fed into the reactor, FL-PY, with a 4:1 ratio of methane to coal (Steinberg, 1986). The coal will be mixed with a natural gas stream, REACFEED Table 2, containing approximately 96% methane, 2% ethane, 0.6% propane, 0.26% butane, 0.2% pentane, 0.1% hexane, and 0.8% heptane (Faramawy, 2016). The reaction for the flash pyrolysis of coal in an atmosphere of methane can be broken down into two different general reactions.



2 Methane => Ethylene + 2 H<sub>2</sub>

Coal + H<sub>2</sub> => CO<sub>2</sub> + CO + Methane + Ethane + BTX

The process is run at 1832 °F and 500 Psia to maximize the yields of valuable products. According to Steinberg, residence times of 1.5 seconds or less are needed to provide a yield of 8% ethylene, 6% BTX and 79% char from the dry coal. The stream, PYROLP Table 2, coming out of FL-PY is immediately quenched, QUENCH, with water to cool down to 400 °F. This prevents the product stream from further reacting and producing undesirable products. The quenched product stream, QNCHO Table 2, is then processed through a plate and frame separator, SOLSEP, with an aluminum plate to remove the solid char from the gaseous products. Plate and frame separators operate by moving a solid-gas stream through a filter plate where the solid char particles accumulate. As the “cake” of char accumulates, the filter resistance increases. Therefore, a second plate and frame separator is required to divert the flow of the stream to another plate and frame separator while cleaning out the filter plates of the one that just ran. An assumption is made that SOLSEP is operating adiabatically. This assumption would require sufficient insulation to minimize heat loss. The char, CHAR Table 3, is collected from the filters and used to satisfy the heating requirements of the process. According to Kang et. al, the heating value of char is 11091 Btu/lb. This accounts for all the heating required for FL-PY excluding start-up due to not being available yet. The gas stream, SEPO Table 3, is fed through 30 gasketed plate heat exchangers, COOL, in parallel and cooled to 70 °F with 60 °F water. A gasketed plate heat exchanger uses metal plates to transfer heat between two fluids. The cooled stream, COOLOUT Table 4, is fed through a flash unit, FLASH1, to separate water from the gas stream. The flash unit involves using a partial liquid gas stream and creating an interface where the liquid comes out the bottom and the gas comes out the top. The liquid stream, WATEROUT Table 4, which contains phenols and other impurities is sent to a waste water plant to be treated. The top stream, PRODUCTS Table 4, is sent to a heat exchanger, TURBHEAT, to heat the stream to 150 °F. This is done so that the stream is above the dew point upon entering the turboexpander, TURB. A turboexpander is a centrifugal turbine that high-pressure gas enters and is expanded. This process expands the gas from 500 psi to 14.7 psi and lowers the temperature to -84.7 °F. Additionally, from the expansion of the gas, work is being produced. This work can be used to minimize the amount of electricity that needs to be purchased. The stream, LOWP Table 5, coming out of TURB is sent into a flash unit, FLASH2, that separates most of the FG from the BTX stream. The FG is then sent to a heat exchanger, RECHEAT, and heated to 70 °F. The stream, SPLITIN Table 6, is then split into two streams. The first is PURGE Table 6, which is a purge stream. The other stream REC Table 6, is the remainder after being split and is recycled to FL-PY where it is mixed with REACFEED Table 2. PURGE removes 50% of the stream from SPLITIN. This is done to maintain at least a 0.8 mass fraction of methane entering the reactor. Since 50% of the stream is removed, a make-up stream of natural gas, NATGAS Table 6, is mixed with the recycle stream and fed into the reactor. PURGE will be burned to meet the heating requirements of the plant not being satisfied by the solid char. The liquid stream out of FLASH2 is fed into DISTHEAT which is a heat exchanger that heats the stream to 70 °F. DISTFEED, Table 7, is then fed into a distillation column, DIST, to remove the remaining FG from the mixed BTX stream. The tower is operating at 14.7 psi and the condenser is operating at

58 °F, requiring cooling, and the reboiler is operating at 200.5 °F. The FG stream coming out of the distillate will be burned to meet the heating requirements of the plant not being satisfied by the solid char. The HEPBTX stream will be fed through a pump, PUMP, to re-pressurize it to 200 psig. The pressure is changed to match the pressure of the extractor, EXTRACT, to conduct the separation of BTX from heptane and hexane using liquid-liquid extraction. EXTRACT uses a variety of moving parts to mix the two streams and operates at a range of pressures of 75 psi at stage 1, 135 psi at stage 30 and 200 at stage 60 as specified by Forte et al. The temperature is set to 260 °F. The solvent used is tetraethylene glycol. The two liquid streams will come out of the extractor. RAFIN, Table 8, will be a mixed stream of heptane and hexane and a small amount of the solvent. It is sent to a distillation column, RECOV2, to separate the heptane and hexane from the solvent. The RAFGAS containing heptane and hexane is sold as “raffinate.” The solvent, RECSOL2 Table 9, will be recycled and reused in EXTRACT. The other liquid stream, BOTTOMS Table 10, coming out of EXTRACT is sent to a distillation column, RECOVERY, to separate the tetraethylene glycol from the BTX. The BTX stream will be essentially pure and can be sold. The tetraethylene glycol stream will be mixed and recycled and added with a makeup stream to be refeed into EXTRACT.

Several assumptions were necessary to simulate the process. The first of these assumptions is that the simulated reactor provides the same yields and yield distribution that were observed by Steinberg (Steinberg, 1986). This assumption provided a basis for the composition of the product stream used in the simulation. Another necessary assumption was that the plate and frame separator removes 100% of the solid char that exits the reactor from the product stream. This assumption was necessary as the process requires distillation downstream, which generally does not involve solids. A third assumption used for the design of the process is that heavy tars and other organic compounds are present in small amounts in the pyrolysis product stream and that these heavy compounds exit FLASH 1 with the water stream. This assumption was needed because of the lack of pertinent information on the subject. Another necessary assumption made is that a gaseous reactor feed of 80% methane is sufficient for the reactor to provide the desired products at the levels cited in the literature. This assumption was necessary to determine the amount of the recycle stream needed to be purged before reentering the reactor. The cryogenic turboexpander is also assumed to run at isentropic conditions. This assumption is necessary as there is no information available to calculate an isentropic efficiency. It is also assumed that a water treatment plant will be available for the removal of the water contaminants so that the water can be reused in the process. Another approximation used in the simulation is the efficiency of the trays in the distillation towers. An efficiency of 80% was assumed for the trays in order to size and price the distillation columns. Another assumption used was that the EXTRACT column is capable of a liquid-liquid extraction in which BTX is recovered at the rates described in US Patent 4,690,733. It was also assumed that roughly 10% of the solvent exits the extraction column with the raffinate. One more assumption that was necessary to make was that this plant will exist near a plant having need of the excess fuel gas that is produced in the process. This is necessary since the fuel gas stream that ends up being collected would not be permitted to reenter a natural gas pipeline. The last approximation necessary for the process design was that there is minimal pressure loss across the process. The equipment is designed to

operate at 500 psia and it is assumed that the pressure drop throughout the process does not significantly lower this pressure.

The design of this process began with the reactor design. The composition of the reactor effluent was the basis for the entire process design. Once this composition had been defined, it was necessary to implement the separation processes. The first of the components that needed to be removed was the char from the pyrolysis reaction. This was necessary as solid flow through a chemical process can damage equipment and cause significant flow problems if the solid coagulates. The solution to this problem was to incorporate a solid separation filter. This filter allows the char to collect on the surface of the filter while the remaining gases continue through the process. Because a large amount of water is used to quench the system, the water and the organic compounds need to be separated. To do this, a flash separator was used. The difference in vapor pressures between water and the desired organic compounds was significant enough to flash the organic compounds from the water, leaving only a small amount of water in the organic phase. The next separation necessary in the process was the removal of methane and other light components from the heavier organics. Because the product stream is a gaseous stream at high pressures, it was possible to implement a cryogenic turboexpander to isentropically reduce the pressure of the products, causing the heavier components to condense at the resulting lower temperatures. With the heavier compounds now in the liquid phase, it was necessary to introduce another flash unit for the separation of these compounds from the gaseous components that did not condense during the expansion process. The lighter gases could then be recompressed and recycled into the reactor. A recycle stream was introduced to limit the amount of natural gas that needed to be purchased. A purge stream was introduced to keep the methane mass fraction above 0.8. The remaining liquid components consisted mostly of hydrocarbon compounds with at least three carbons. With significantly different boiling points between the lighter hydrocarbons and the heavier hydrocarbons, a distillation tower was introduced to split the pentanes and lighter components from the hexanes, heptanes, and aromatics. The lighter components can be used to heat processes in the system or be sold for heating value. Because of the similarity of boiling points between hexane, heptane, and the aromatics, a flash unit or distillation tower would not be sufficient to separate these compounds. In order to successfully separate the linear hydrocarbons from the aromatics, a solvent extraction process was introduced. Tetraethylene glycol was recommended by US Patent 4,690,733 and was used to extract the aromatics from the other compounds. Because tetraethylene glycol has a much higher boiling point than any of the other components, the aromatics and lighter hydrocarbons could be distilled from the solvent and it could be recycled. After the final distillation, there is an almost pure aromatic stream and an almost pure stream of hexane and heptane.

Figure 1 displays the representative flowsheet for the process of the separation of the products from the flash pyrolysis of coal in an atmosphere of methane.

Figure 1. Aspen+ simulation model.

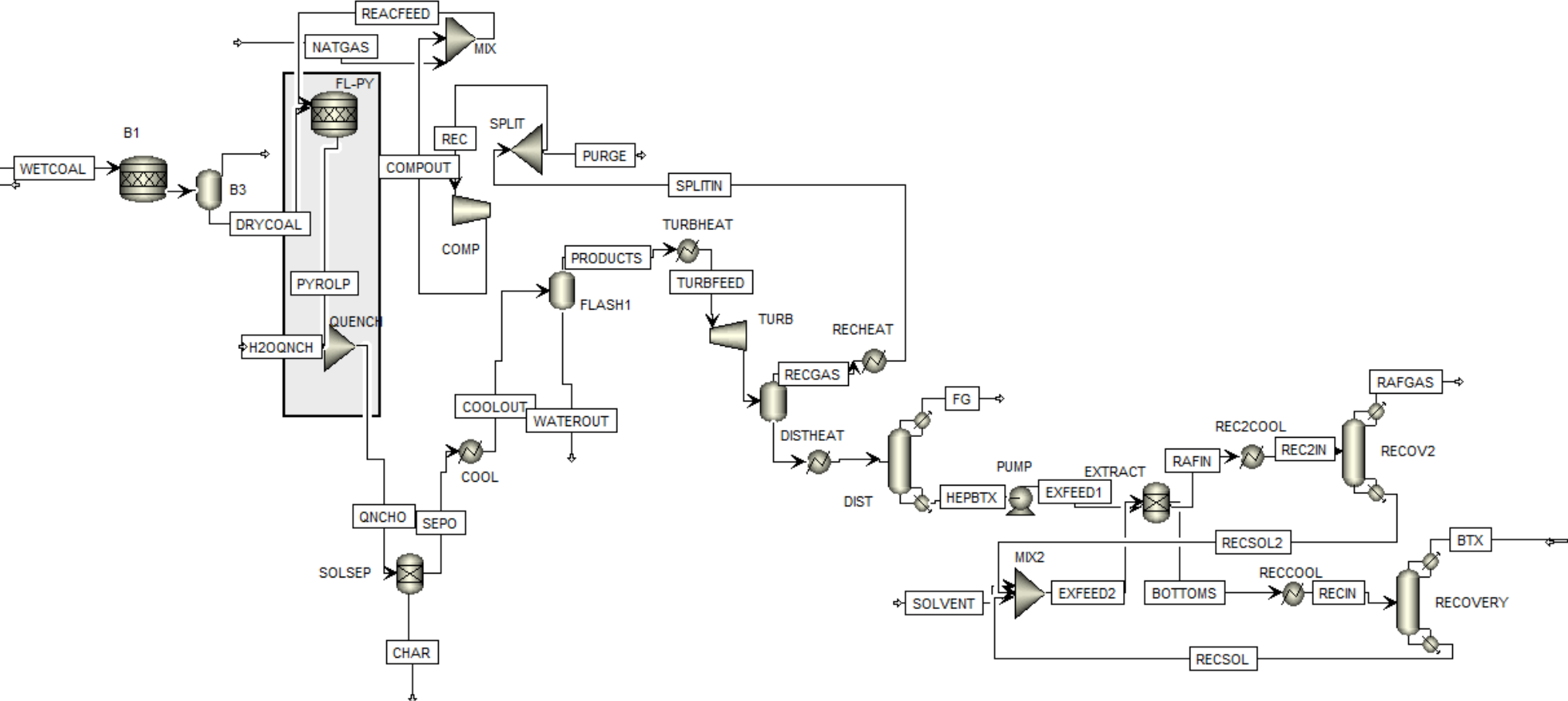
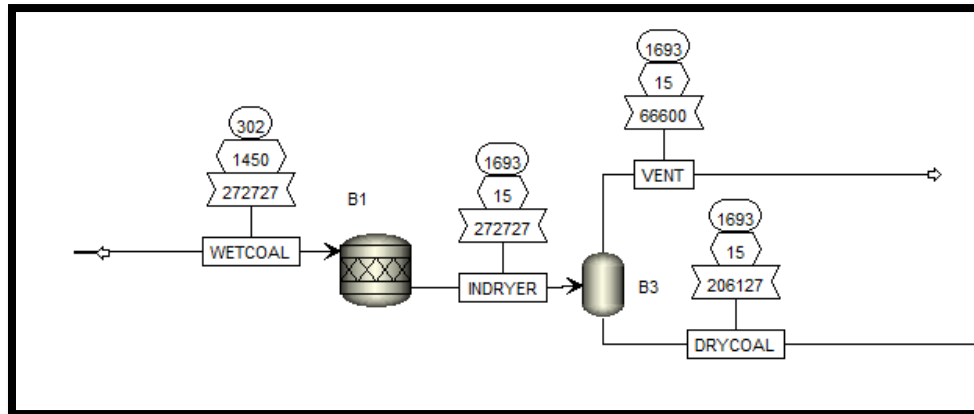


Figure 2 shows the dryer unit as modeled in Aspen.



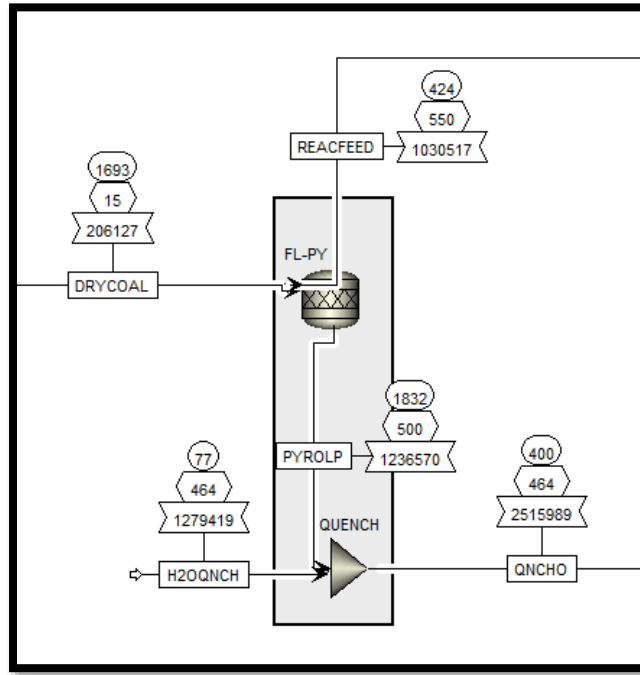
**Figure 2. Dryer Unit**

The dryer unit receives feed from a grinder unit which is not displayed. In order to model the drying of the coal, the coal must be fed to a reactor and the moisture in the coal must be converted to gaseous water. This water is then flashed off in the second part of the modelling unit. In reality, this would be a single dryer unit.

**Table 1. Stream table for Grinding and Dryer Unit.**

	<b>Units</b>	<b>ROM</b>	<b>INDRYER</b>	<b>VENT</b>	<b>DRYCOAL</b>
<b>Description</b>					
<b>From</b>			DRYER1	DRYER2	DRYER2
<b>To</b>		DRYER1	DRYER2		FL-PY
<b>Stream Class</b>		MIXNC	MIXNC	MIXNC	MIXNC
<b>Total Stream</b>					
<b>Temperature</b>	F	302	1693	1693	1693
<b>Pressure</b>	psia	1450	14.7	14.7	14.7
<b>Mass Vapor Fraction</b>		0	0.2442	1	0
<b>Mass Liquid Fraction</b>		0	0	0	0
<b>Mass Solid Fraction</b>		1	0.7558	0	1
<b>Mass Enthalpy</b>	Btu/lb	-2554	-2554	-4952	-1779
<b>Mass Density</b>	lb/cuft	85.074	0.047	0.011	85.074
<b>Enthalpy Flow</b>	Btu/hr	- 696,517,046	- 696,517,046	- 329,778,209	- 366,738,838
<b>Mass Flows</b>	lb/hr	272,727	272,727	66,600	206,127
CO	lb/hr	0	0	0	0
CO2	lb/hr	0	0	0	0
H2O	lb/hr	0	66,600	66,600	0
C1P	lb/hr	0	0	0	0
C2P	lb/hr	0	0	0	0
C2O	lb/hr	0	0	0	0
BENZENE	lb/hr	0	0	0	0
TOLUENE	lb/hr	0	0	0	0
C8AROM	lb/hr	0	0	0	0
COAL	lb/hr	272,727	206,127	0	206,127
<b>Mass Fractions</b>					
CO		0	0	0	0
CO2		0	0	0	0
H2O		0	0.244	1	0
C1P		0	0	0	0
C2P		0	0	0	0
C2O		0	0	0	0
BENZENE		0	0	0	0
TOLUENE		0	0	0	0
C8AROM		0	0	0	0
COAL		1	0.756	0	1

Figure 3 displays the reactor and quench. This unit consists of a reactor with a dry coal and gas feed and a mixing block.



**Figure 3. Reactor and Quench**

The reactor is fed streams of dry coal and a natural gas and recycle gas mixture. The products from the reactor are quickly quenched with a substantial amount of water to bring the products down to a temperature at which the pyrolysis reactions cease.

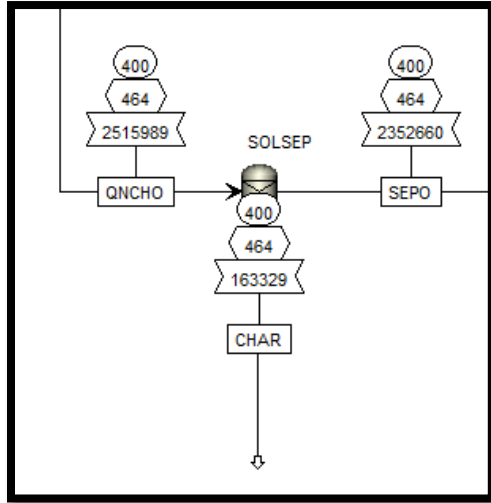
**Table 2. Stream table for the Reactor – Flash Pyrolizer Unit.**

	<b>Units</b>	<b>DRYCOAL</b>	<b>REACFEED</b>	<b>PYROLP</b>	<b>H2OQNCH</b>	<b>QNCHO</b>
<b>Description</b>						
<b>From</b>		B3	MIX	FL-PY		QUENCH
<b>To</b>		FL-PY	FL-PY	QUENCH	QUENCH	SOLSEP
<b>Temperature</b>	F	1693	424	1832	77	400
<b>Pressure</b>	psia	14.7	550	500	464	464
<b>Mass Vapor Fraction</b>		0	1	0.8679	0	0.9351
<b>Mass Liquid Fraction</b>		0	0	0	1	0
<b>Mass Solid Fraction</b>		1	0	0.1321	0	0.06492
<b>Mass Enthalpy</b>	Btu/lb	-1779.19	-1611.53	-231.60	-6892.09	-3618.56
<b>Mass Density</b>	lb/cuft	85.07	1.06	0.43	47.20	1.05
<b>Enthalpy Flow</b>	Btu/hr	-366738838	-1660705037	-286392248	-8817870251	-9104262503
<b>Mass Flows</b>	lb/hr	206127	1030517	1236570	1279419	2515989
CO	lb/hr	0	16331	32663	0	32663
CO2	lb/hr	0	5430	10885	0	10885
H2O	lb/hr	0	160	160	1279419	1279578
C1P	lb/hr	0	824508	824508	0	824508
C2P	lb/hr	0	67431	67542	0	67542
C2O	lb/hr	0	12225	24503	0	24503
C3P	lb/hr	0	28601	28601	0	28601
BENZENE	lb/hr	0	51.25	3149	0	3149
TOLUENE	lb/hr	0	4.67	2929	0	2929
C8AROM	lb/hr	0	0.41	2527	0	2527
COAL	lb/hr	206127	0	163329	0	163329
N-BUT-01	lb/hr	0	6065	6065	0	6065
ISOBU-01	lb/hr	0	10033	10033	0	10033
2-MET-01	lb/hr	0	6814	6814	0	6814
N-PEN-01	lb/hr	0	2755	2755	0	2755
N-HEX-01	lb/hr	0	4927	4927	0	4927
N-HEP-01	lb/hr	0	45179	45179	0	45179
TETRA-01	lb/hr	0	0	0	0	0



	<b>Units</b>	<b>DRYCOAL</b>	<b>REACFEED</b>	<b>PYROLP</b>	<b>H2OQNCH</b>	<b>QNCHO</b>
<b>Mass Fractions</b>						
CO		0	0.01585	0.02641	0	0.01298
CO2		0	0.00527	0.00880	0	0.00433
H2O		0	0.00015	0.00013	1	0.50858
C1P		0	0.80009	0.66677	0	0.32771
C2P		0	0.06543	0.05462	0	0.02684
C2O		0	0.01186	0.01982	0	0.00974
C3P		0	0.02775	0.02313	0	0.01137
BENZENE		0	0.00005	0.00255	0	0.00125
TOLUENE		0	0.00000	0.00237	0	0.00116
C8AROM		0	0.00000	0.00204	0	0.00100
COAL		1	0.00000	0.13208	0	0.06492
N-BUT-01		0	0.00589	0.00490	0	0.00241
ISOBU-01		0	0.00974	0.00811	0	0.00399
2-MET-01		0	0.00661	0.00551	0	0.00271
N-PEN-01		0	0.00267	0.00223	0	0.00109
N-HEX-01		0	0.00478	0.00398	0	0.00196
N-HEP-01		0	0.04384	0.03654	0	0.01796
TETRA-01		0	0	0	0	0

Figure 4 shows the filter used to separate the char from the gaseous products from the reaction. In order to effectively model the process, a Separation block is used to completely separate the char from the other components.



**Figure 4. Filter for Solid Separation**

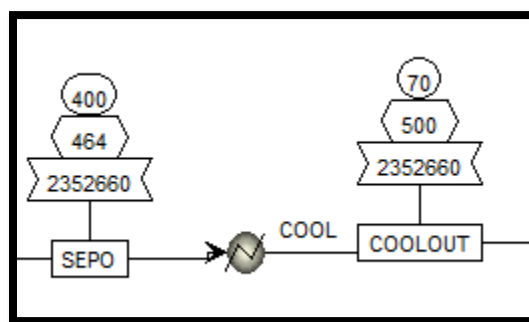
The filter shown in Figure 4 removes the solid char from the quenched reactor product stream. The reactor has considerable heating requirements, so the resulting char from the filter is combusted to provide enough heat for the process. The gases pass through SOLSEP and are processed more downstream.

**Table 3. Stream table for Solid Separator and Conveyer Unit.**

	<b>Units</b>	<b>QNCHO</b>	<b>CHAR</b>	<b>SEPO</b>
<b>Description</b>				
<b>From</b>		QUENCH	SOLSEP	SOLSEP
<b>To</b>		SOLSEP		COOL
<b>Temperature</b>	F	400	400	400
<b>Pressure</b>	psia	464	464	464
<b>Mass Vapor Fraction</b>		0.9351	0	1
<b>Mass Liquid Fraction</b>		0	0	0
<b>Mass Solid Fraction</b>		0.06492	1	0
<b>Mass Enthalpy</b>	Btu/lb	-3619	-953	-3804
<b>Mass Density</b>	lb/cuft	1.048	85.074	0.981
<b>Enthalpy Flow</b>	Btu/hr	-9104262503	-155652939	-8948609564
<b>Mass Flows</b>	lb/hr	2515989	163329	2352660
CO	lb/hr	32663	0	32663
CO2	lb/hr	10885	0	10885
H2O	lb/hr	1279578	0	1279578
C1P	lb/hr	824508	0	824508
C2P	lb/hr	67542	0	67542
C2O	lb/hr	24503	0	24503
C3P	lb/hr	28601	0	28601
BENZENE	lb/hr	3149	0	3149
TOLUENE	lb/hr	2929	0	2929
C8AROM	lb/hr	2527	0	2527
COAL	lb/hr	163329	163329	0
N-BUT-01	lb/hr	6065	0	6065
ISOBU-01	lb/hr	10033	0	10033
2-MET-01	lb/hr	6814	0	6814
N-PEN-01	lb/hr	2755	0	2755
N-HEX-01	lb/hr	4927	0	4927
N-HEP-01	lb/hr	45179	0	45179
TETRA-01	lb/hr	0	0	0

	Units	QNCHO	CHAR	SEPO
<b>Mass Fractions</b>				
CO		0.01298	0	0.01388
CO2		0.00433	0	0.00463
H2O		0.50858	0	0.54389
C1P		0.32771	0	0.35046
C2P		0.02684	0	0.02871
C2O		0.00974	0	0.01042
C3P		0.01137	0	0.01216
BENZENE		0.00125	0	0.00134
TOLUENE		0.00116	0	0.00125
C8AROM		0.00100	0	0.00107
COAL		0.06492	1	0
N-BUT-01		0.00241	0	0.00258
ISOBU-01		0.00399	0	0.00426
2-MET-01		0.00271	0	0.00290
N-PEN-01		0.00109	0	0.00117
N-HEX-01		0.00196	0	0.00209
N-HEP-01		0.01796	0	0.01920
TETRA-01		0	0	0

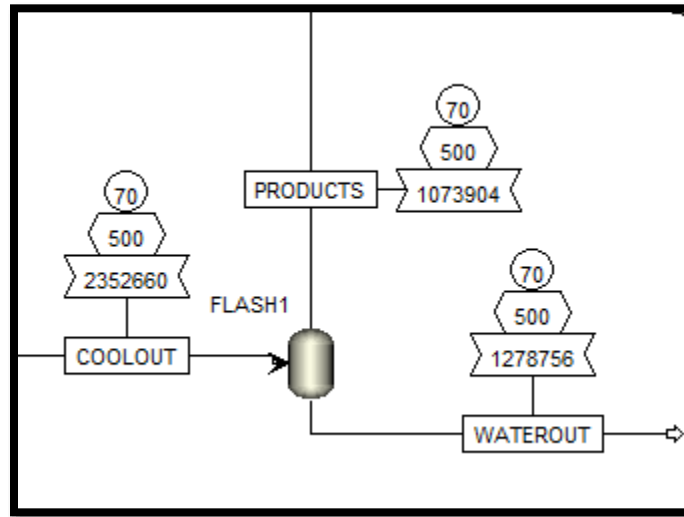
Figure 5 shows a simplified model of the coolers necessary to condense the water and contaminants such as phenols, cresols, and xylenols that will be present in small amounts in the stream.



**Figure 5. Cooler**

COOL shown in Figure 5 is a simplified model of a group of heat exchangers using cooling water to decrease the temperature of the gaseous stream. This decrease in temperature is necessary to condense some of the heavier components of the stream so that a flash unit downstream can make a successful separation of these components.

A flash unit is displayed in Figure 6 that is used to separate the majority of the water and its contaminants from the more valuable products to be recovered from the pyrolysis process.



**Figure 6. Flash Unit 1**

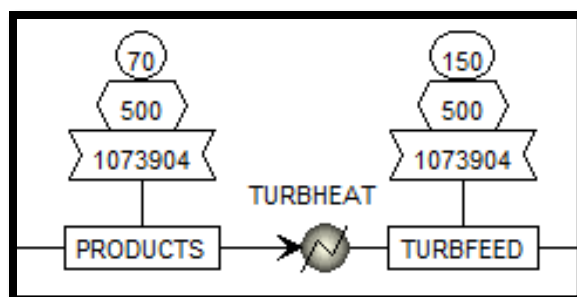
A large portion of the flow from the quench consisted of water. After being cooled, this water can be flashed from the other components which have not condensed. The gaseous products from FLASH1 consist mostly of straight-chain hydrocarbons and some aromatics.

**Table 4. Stream table for Cooler and Flash Separator Unit 1.**

	<b>Units</b>	<b>SEPO</b>	<b>COOLOUT</b>	<b>WATEROUT</b>	<b>PRODUCTS</b>
<b>Description</b>					
<b>From</b>		SOLSEP	COOL	FLASH1	FLASH1
<b>To</b>		COOL	FLASH1		TURBHEAT
<b>Temperature</b>	F	400	70	70	70
<b>Pressure</b>	psia	464	500	500	500
<b>Mass Vapor Fraction</b>		1	0.4565	0	1
<b>Mass Liquid Fraction</b>		0	0.5435	1	0
<b>Mass Solid Fraction</b>		0	0	0	0
<b>Mass Enthalpy</b>	Btu/lb	-3804	-4568	-6900	-1792
<b>Mass Density</b>	lb/cuft	0.981	3.721	47.328	1.774
<b>Enthalpy Flow</b>	Btu/hr	-8948609564	-10747735277	-8823337868	-1924397410
<b>Mass Flows</b>	lb/hr	2352660	2352660	1278756	1073904
CO	lb/hr	32663	32663	0	32663
CO2	lb/hr	10885	10885	8	10877
H2O	lb/hr	1279578	1279578	1278732	846
C1P	lb/hr	824508	824508	14	824494
C2P	lb/hr	67542	67542	1	67540
C2O	lb/hr	24503	24503	1	24502
C3P	lb/hr	28601	28601	0	28601
BENZENE	lb/hr	3149	3149	1	3149
TOLUENE	lb/hr	2929	2929	0	2929
C8AROM	lb/hr	2527	2527	0	2527
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	6065	6065	0	6065
ISOBU-01	lb/hr	10033	10033	0	10033
2-MET-01	lb/hr	6814	6814	0	6814
N-PEN-01	lb/hr	2755	2755	0	2755
N-HEX-01	lb/hr	4927	4927	0	4927
N-HEP-01	lb/hr	45179	45179	0	45179
TETRA-01	lb/hr	0	0	0	0

	Units	SEPO	COOLOUT	WATEROUT	PRODUCTS
<b>Mass Fractions</b>					
CO		0.01388	0.01388	0.00000	0.03042
CO2		0.00463	0.00463	0.00001	0.01013
H2O		0.54389	0.54389	0.99998	0.00079
C1P		0.35046	0.35046	0.00001	0.76775
C2P		0.02871	0.02871	0.00000	0.06289
C2O		0.01042	0.01042	0.00000	0.02282
C3P		0.01216	0.01216	0.00000	0.02663
BENZENE		0.00134	0.00134	0.00000	0.00293
TOLUENE		0.00125	0.00125	0.00000	0.00273
C8AROM		0.00107	0.00107	0.00000	0.00235
COAL		0	0	0	0
N-BUT-01		0.00258	0.00258	0	0.00565
ISOBU-01		0.00426	0.00426	0	0.00934
2-MET-01		0.00290	0.00290	0	0.00635
N-PEN-01		0.00117	0.00117	0	0.00257
N-HEX-01		0.00209	0.00209	0	0.00459
N-HEP-01		0.01920	0.01920	0	0.04207
TETRA-01		0	0	0	0

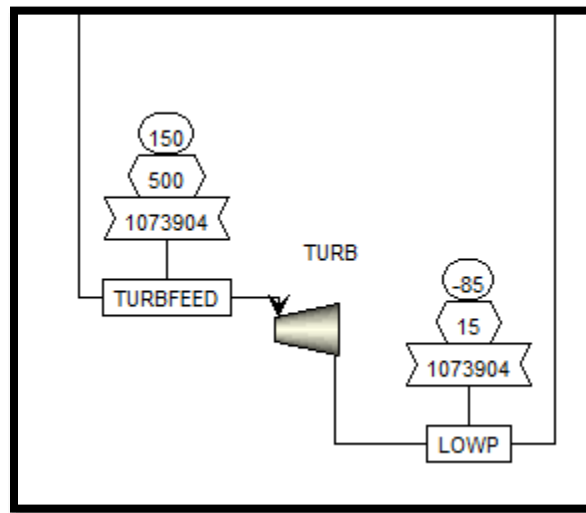
Figure 7 displays a heater used to raise the temperature of the gaseous stream from the flash unit.



**Figure 7. Post-flash Heater**

TURBHEAT depicted in Figure 7 is necessary to keep the gaseous stream above its dew point when entering in the cryogenic turboexpander downstream. The turboexpander requires that its feed is completely gaseous, so this heater is necessary to achieve this.

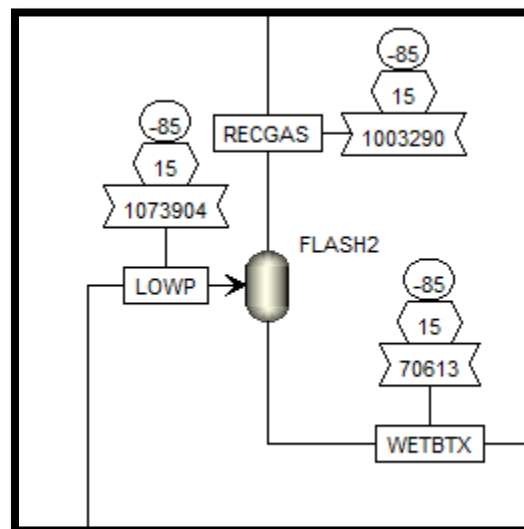
Figure 8 shows the cryogenic turboexpander used to condense a portion of the gaseous stream.



**Figure 8. Cryogenic Turboexpander**

TURB is used to drastically decrease the pressure of the gaseous flow. This is accomplished by having the gas flow through a large turbine. As the gas causes the turbine to spin, electricity is produced and the gas depressurizes. This expansion of the gas greatly reduces the temperature of the gas, resulting in the condensation of some of the heavier compounds found in the gas.

Figure 9 presents the second flash unit in the process. This flash unit separates the heavier components like hexane and BTX from the lighter compounds that did not condense during the cryogenic turboexpansion process.



**Figure 9. Flash Unit 2**



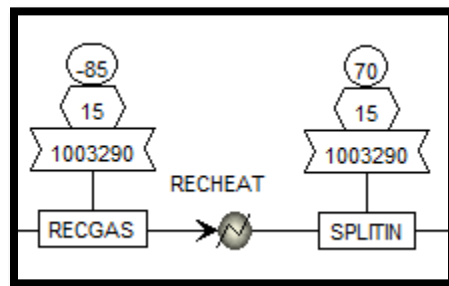
FLASH2 is necessary to separate gas that will be recycled to the reactor and heavier liquids that will be purified and sold. The gas to be recycled consists mostly of methane with some impurities. The liquid stream from the flash unit has considerable amounts of straight-chain alkanes with some aromatics.

**Table 5. Stream table for Post Flash Heater Turbo Expander and Flash Separator Unit 2.**

	<b>Units</b>	<b>PRODUCTS</b>	<b>TURBFEED</b>	<b>LOWP</b>	<b>RECGAS</b>	<b>WETBTX</b>
<b>Description</b>						
<b>From</b>		FLASH1	TURBHEAT	TURB	FLASH2	FLASH2
<b>To</b>		TURBHEAT	TURB	FLASH2	RECHEAT	DISTHEAT
<b>Temperature</b>	F	70	150	-85	-85	-85
<b>Pressure</b>	psia	500	500	14.7	14.7	14.7
<b>Mass Vapor Fraction</b>		1	1	0.9342461	1	0
<b>Mass Liquid Fraction</b>		0	0	0.0657539	0	1
<b>Mass Solid Fraction</b>		0	0	0	0	0
<b>Mass Enthalpy</b>	Btu/lb	-1792	-1747	-1860	-1922	-979
<b>Mass Density</b>	lb/cuft	1.7742	1.4826	0.0695	0.0650	41.0468
<b>Enthalpy Flow</b>	Btu/hr	-1924397410	-1876254076	-1997333628	-1928188698	69144929.88
<b>Mass Flows</b>	lb/hr	1073904	1073904	1073904	1003290	70613
CO	lb/hr	32663	32663	32663	32662	1.3
CO2	lb/hr	10877	10877	10877	10861	17
H2O	lb/hr	846	846	846	319	527
C1P	lb/hr	824494	824494	824494	824353	142
C2P	lb/hr	67540	67540	67540	67227	314
C2O	lb/hr	24502	24502	24502	24451	52
C3P	lb/hr	28601	28601	28601	27446	1155
BENZENE	lb/hr	3149	3149	3149	102	3046
TOLUENE	lb/hr	2929	2929	2929	9	2920
C8AROM	lb/hr	2527	2527	2527	1	2526
COAL	lb/hr	0	0	0	0	0
N-BUT-01	lb/hr	6065	6065	6065	4286	1779
ISOBU-01	lb/hr	10033	10033	10033	8299	1733
2-MET-01	lb/hr	6814	6814	6814	2268	4546
N-PEN-01	lb/hr	2755	2755	2755	641	2114
N-HEX-01	lb/hr	4927	4927	4927	163	4765
N-HEP-01	lb/hr	45179	45179	45179	203	44977
TETRA-01	lb/hr	0	0	0	0	0

	Units	PRODUCTS	TURBFEED	LOWP	RECGAS	WETBTX
<b>Mass Fractions</b>						
CO		0.0304	0.0304	0.0304	0.0326	0.0000
CO2		0.0101	0.0101	0.0101	0.0108	0.0002
H2O		0.0008	0.0008	0.0008	0.0003	0.0075
C1P		0.7678	0.7678	0.7678	0.8216	0.0020
C2P		0.0629	0.0629	0.0629	0.0670	0.0044
C2O		0.0228	0.0228	0.0228	0.0244	0.0007
C3P		0.0266	0.0266	0.0266	0.0274	0.0164
BENZENE		0.0029	0.0029	0.0029	0.0001	0.0431
TOLUENE		0.0027	0.0027	0.0027	0.0000	0.0413
C8AROM		0.0024	0.0024	0.0024	0.0000	0.0358
COAL		0	0	0	0	0
N-BUT-01		0.0056	0.0056	0.0056	0.0043	0.0252
ISOBU-01		0.0093	0.0093	0.0093	0.0083	0.0245
2-MET-01		0.0063	0.0063	0.0063	0.0023	0.0644
N-PEN-01		0.0026	0.0026	0.0026	0.0006	0.0299
N-HEX-01		0.0046	0.0046	0.0046	0.0002	0.0675
N-HEP-01		0.0421	0.0421	0.0421	0.0002	0.6369
TETRA-01		0	0	0	0	0

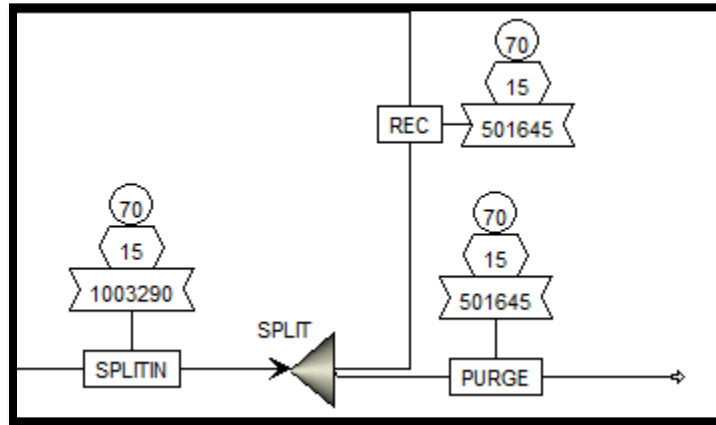
Figure 10 displays a heater used to raise the temperature of the recycle gas to a temperature at which it can be re-compressed.



**Figure 10. Recycle Gas Heater**

Because the gas must be re-compressed, the gas must be at a viable temperature for this process. REHEAT will likely use fuel gas combustion to heat the recycled gases.

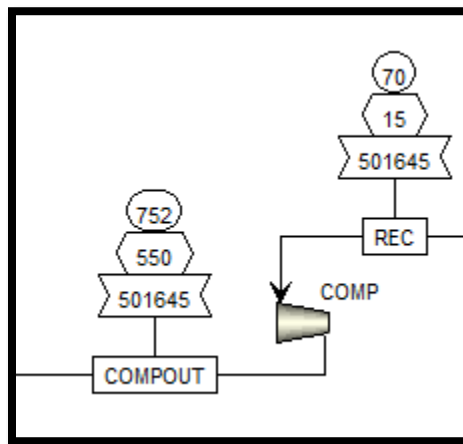
Figure 11 depicts SPLIT which is used to purge a portion of the recycle gas. This is necessary to maintain high levels of methane in the reactor.



**Figure 11. Recycle Gas Splitter**

In order to maintain reactor feed gas methane levels at high levels, some of the recycle gas must be purged to be replaced by natural gas. 50% of the recycle gas is purged and is used for the heating requirements of the plant. The remaining recycle gas is mixed with natural gas to be fed to the reactor. The gaseous feed to the reactor consists of 80% methane, which is assumed to be a sufficiently high enough level of methane for the reaction to produce the desired products.

Figure 12 shows the compressor used to compress the recycle gas up to pressures high enough to be fed to the reactor.

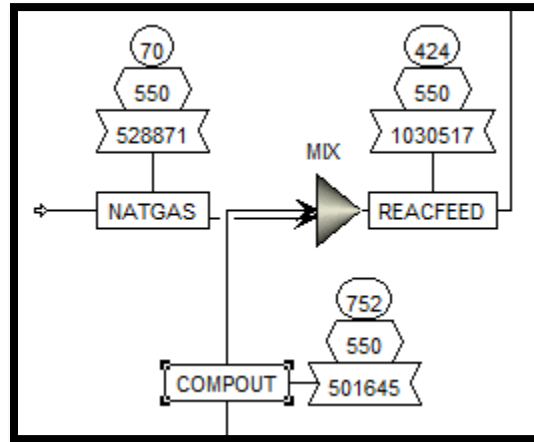


**Figure 12. Recycle Gas Compressor**

As the reactor operates at high pressures, the feed to the reactor must be at least as high of pressures to enter the process. Because the recycle gas is essentially at ambient pressures, it must

be compressed to as high of a pressure as the reactor. COMP increases the recycle gas pressure from roughly ambient to 550 psi.

Figure 13 presents the mixer used to mix the natural gas stream and the recycle gas stream to be fed to the reactor.



**Figure 13. Reactor Feed Mixer**

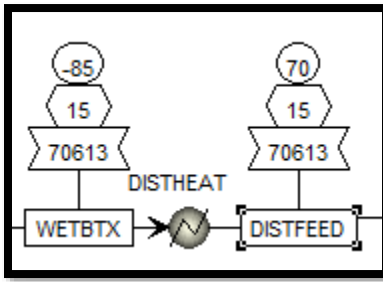
MIX is used to combine the recycle gases and the natural gas to provide feed to the reactor. After being mixed, the resulting gas is roughly 80% methane by weight. This composition of gas is assumed to be sufficient to provide the cited product compositions.

**Table 6. Stream table for Recycle Stream.**

	<b>Units</b>	<b>RECGAS</b>	<b>SPLITIN</b>	<b>PURGE</b>	<b>REC</b>	<b>COMPOUT</b>	<b>NATGAS</b>	<b>REACFEED</b>
<b>Description</b>								
<b>From</b>		FLASH2	RECHEAT	SPLIT	SPLIT	COMP		MIX
<b>To</b>		RECHEAT	SPLIT		COMP	MIX	MIX	FL-PY
<b>Temperature</b>	F	-85	70	70	70	752	70	424
<b>Pressure</b>	psia	14.7	14.7	14.7	14.7	550	550	550
<b>Mass Vapor Fraction</b>		1	1	1	1	1	0.9072	1
<b>Mass Liquid Fraction</b>		0	0	0	0	0	0.0928	0
<b>Mass Enthalpy</b>	Btu/lb	-1922	-1847	-1847	-1847	-1406	-1806	-1612
<b>Mass Density</b>	lb/cuft	0.06496	0.04577	0.04577	0.04577	0.73664	2.01923	1.05542
<b>Enthalpy Flow</b>	Btu/hr	-1928188698	-1853322993	-926661496.3	-926661496.3	-705447195.2	-955257841.5	-1660705037
<b>Mass Flows</b>	lb/hr	1003290	1003290	501645	501645	501645	528871	1030517
CO	lb/hr	32662	32662	16331	16331	16331	0	16331
CO2	lb/hr	10861	10861	5430	5430	5430	0	5430
H2O	lb/hr	319	319	160	160	160	0	160
C1P	lb/hr	824353	824353	412176	412176	412176	412332	824508
C2P	lb/hr	67227	67227	33613	33613	33613	33818	67431
C2O	lb/hr	24451	24451	12225	12225	12225	0	12225
C3P	lb/hr	27446	27446	13723	13723	13723	14878	28601
BENZENE	lb/hr	102.5	102.5	51.2	51.2	51.2	0	51.2
TOLUENE	lb/hr	9.3	9.3	4.7	4.7	4.7	0	4.7
C8AROM	lb/hr	0.8	0.8	0.4	0.4	0.4	0	0.4
N-BUT-01	lb/hr	4286	4286	2143	2143	2143	3922	6065
ISOBU-01	lb/hr	8299	8299	4150	4150	4150	5883	10033
2-MET-01	lb/hr	2268	2268	1134	1134	1134	5680	6814
N-PEN-01	lb/hr	641	641	320	320	320	2434	2755
N-HEX-01	lb/hr	163	163	81	81	81	4846	4927
N-HEP-01	lb/hr	203	203	101	101	101	45078	45179

	<b>Units</b>	<b>RECGAS</b>	<b>SPLITIN</b>	<b>PURGE</b>	<b>REC</b>	<b>COMPOUT</b>	<b>NATGAS</b>	<b>REACFEED</b>
<b>Mass Fractions</b>								
CO		0.0326	0.0326	0.0326	0.0326	0.0326	0	0.0158
CO2		0.0108	0.0108	0.0108	0.0108	0.0108	0	0.0053
H2O		0.0003	0.0003	0.0003	0.0003	0.0003	0	0.0002
C1P		0.8216	0.8216	0.8216	0.8216	0.8216	0.7796	0.8001
C2P		0.0670	0.0670	0.0670	0.0670	0.0670	0.0639	0.0654
C2O		0.0244	0.0244	0.0244	0.0244	0.0244	0	0.0119
C3P		0.0274	0.0274	0.0274	0.0274	0.0274	0.0281	0.0278
BENZENE		0.0001	0.0001	0.0001	0.0001	0.0001	0	4.97E-05
TOLUENE		9.31E-06	9.31E-06	9.31E-06	9.31E-06	9.31E-06	0	4.53E-06
C8AROM		8.24E-07	8.24E-07	8.24E-07	8.24E-07	8.24E-07	0	4.01E-07
N-BUT-01		0.00427	0.00427	0.00427	0.00427	0.00427	0.00742	0.00589
ISOBU-01		0.00827	0.00827	0.00827	0.00827	0.00827	0.01112	0.00974
2-MET-01		0.00226	0.00226	0.00226	0.00226	0.00226	0.01074	0.00661
N-PEN-01		0.00064	0.00064	0.00064	0.00064	0.00064	0.00460	0.00267
N-HEX-01		0.00016	0.00016	0.00016	0.00016	0.00016	0.00916	0.00478
N-HEP-01		0.00020	0.00020	0.00020	0.00020	0.00020	0.08523	0.04384

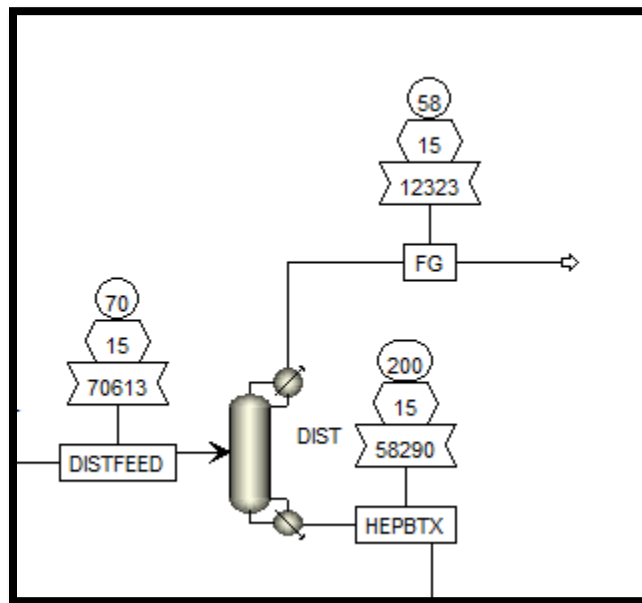
Figure 14 shows DISTHEAT, a heater used to preheat the feed to DIST.



**Figure 14. Distillation Feed Heater**

Because the liquid from FLASH2 is at such a low temperature, it can't be reasonably distilled. To get into a reasonable temperature range for a separation between lighter hydrocarbons and the rest of the liquid, the liquid needs to be heated. This heater will likely use fuel gas combustion to achieve this heating.

Figure 15 displays the distillation tower used to separate some lighter components of the liquid from FLASH2 from the more valuable aromatics and heavier straight-chain hydrocarbons.

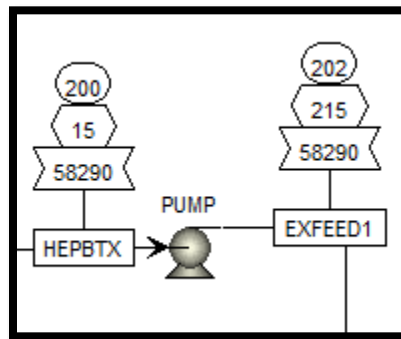


**Figure 15. Light Hydrocarbon Distillation Tower**

DIST is fed a heated liquid stream coming from FLASH2. The purpose of DIST is to remove lighter hydrocarbons from the more valuable hexane, heptane, and BTX. This separation is accomplished based on the differences in boiling points between the lighter and heavier compounds. The reboiler will use fuel gas combustion and the condenser will function with the use of a single-pass refrigeration. The resulting distillate stream can be sold based on its heating value. The liquid stream from DIST receives more processing downstream in order to purify the valuable products.



Figure 16 displays a pump used to increase the pressure of the liquid stream being fed to an extractor.



**Figure 16. Extractor Feed Pump**

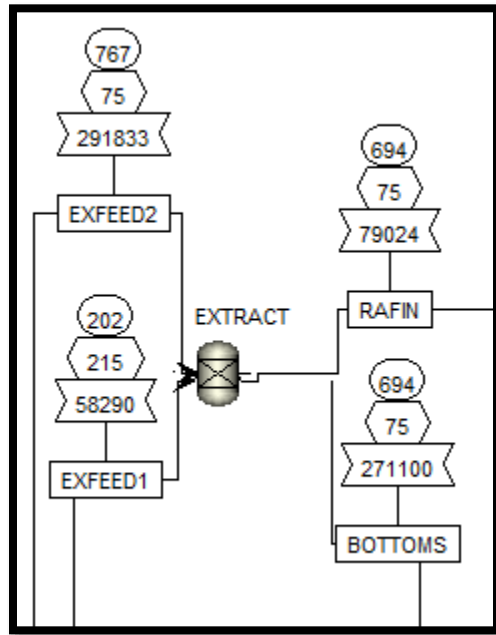
PUMP is necessary to increase the pressure of the liquid feed to the liquid-liquid extractor. This pump is necessary as it is recommended by US Patent 4,690,733 to operate the extractor with a range of 75-200 psi throughout the column. In order to achieve these pressures, the feed to the extractor must have at least as high of pressures.

**Table 7. Stream table for Distillation Column 1 and Pump.**

	<b>Units</b>	<b>DISTFEED</b>	<b>FG</b>	<b>HEPBTX</b>	<b>EXFEED1</b>
<b>Description</b>					
<b>From</b>		DISTHEAT	DIST	DIST	PUMP
<b>To</b>		DIST		PUMP	EXTRACT
<b>Temperature</b>	F	70	58	200	202
<b>Pressure</b>	psia	14.7	14.7	14.7	215
<b>Mass Vapor Fraction</b>		0.019	1	1.61E-08	0
<b>Mass Liquid Fraction</b>		0.981	0	1	1
<b>Mass Solid Fraction</b>		0	0	1.36E-09	0
<b>Mass Enthalpy</b>	Btu/lb	-903	-1165	-745	-744
<b>Mass Density</b>	lb/cuft	4.83	0.15	35.13	35.27
<b>Enthalpy Flow</b>	Btu/hr	-63794856	-14359034	-43442612	-43344098
<b>Mass Flows</b>	lb/hr	70613	12323	58290	58290
CO	lb/hr	1.3	1.3	0	0
CO2	lb/hr	16.5	16.5	0	0
H2O	lb/hr	527	527	0	0
C1P	lb/hr	142	142	0	0
C2P	lb/hr	314	314	0	0
C2O	lb/hr	51.8	51.8	0	0
C3P	lb/hr	1155	1155	0	0
BENZENE	lb/hr	3046	0	3046	3046
TOLUENE	lb/hr	2920	0	2920	2920
C8AROM	lb/hr	2526	0	2526	2526
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	1779	1779	0	0
ISOBU-01	lb/hr	1733	1733	0	0
2-MET-01	lb/hr	4546	4546	0	0
N-PEN-01	lb/hr	2114	2057	56	56
N-HEX-01	lb/hr	4765	0	4765	4765
N-HEP-01	lb/hr	44977	0	44977	44977
TETRA-01	lb/hr	0	0	0	0

	<b>Units</b>	<b>DISTFEED</b>	<b>FG</b>	<b>HEPBTX</b>	<b>EXFEED1</b>
<b>Mass Fractions</b>					
CO		2E-05	1E-04	2E-82	2E-82
CO2		0.0002	0.0013	2E-57	2E-57
H2O		0.0075	0.0427	3E-12	3E-12
C1P		0.0020	0.0115	8E-69	8E-69
C2P		0.0044	0.0255	9E-47	9E-47
C2O		0.0007	0.0042	2E-52	2E-52
C3P		0.0164	0.0937	3E-32	3E-32
BENZENE		0.0431	0	0.0523	0.0523
TOLUENE		0.0413	0	0.0501	0.0501
C8AROM		0.0358	0	0.0433	0.0433
COAL		0	0	0	0
N-BUT-01		0.0252	0.1444	0	0
ISOBU-01		0.0245	0.1407	0	0
2-MET-01		0.0644	0.3689	0	0
N-PEN-01		0.0299	0.1670	0.0010	0.0010
N-HEX-01		0.0675	0	0.0817	0.0817
N-HEP-01		0.6369	0	0.7716	0.7716
TETRA-01		0	0	0	0

Figure 17 shows the liquid-liquid extractor used for the separation of BTX from hexane and heptane.



**Figure 17. Liquid-Liquid Extractor**

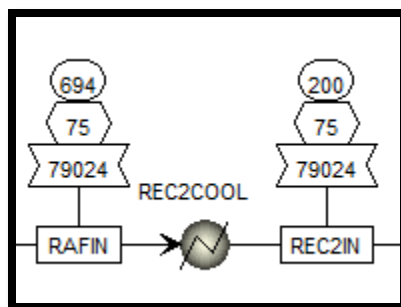
The separation of hexane and heptane from BTX is modeled with a Separation block to simplify the modelling. The separation in EXTRACT is achieved with the use of a tetraethylene glycol solvent. The solvent is fed through the upper portion of the extractor while the products feed is run through the lower portion of the tower. The solvent extracts the BTX from the hexane and heptane and exits through the bottom of the tower. The hexane and heptane exit the top of the tower with a small fraction of the solvent.

**Table 8. Stream table for Extractor.**

	<b>Units</b>	<b>EXFEED1</b>	<b>EXFEED2</b>	<b>RAFIN</b>	<b>BOTTOMS</b>
<b>Description</b>					
<b>From</b>		PUMP	MIX2	EXTRACT	EXTRACT
<b>To</b>		EXTRACT	EXTRACT	REC2COOL	RECCOOL
<b>Temperature</b>	F	202	767	694	694
<b>Pressure</b>	psia	215	75	75	75
<b>Mass Vapor Fraction</b>		0	0.6632	1	0.0064
<b>Mass Liquid Fraction</b>		1	0.3368	0	0.9936
<b>Mass Solid Fraction</b>		0	8.76E-10	0	0
<b>Mass Enthalpy</b>	Btu/lb	-744	-1702	-918	-1762
<b>Mass Density</b>	lb/cuft	35.27	1.92	0.77	30.89
<b>Enthalpy Flow</b>	Btu/hr	-43344098	-496704602	-72551984	-477753929
<b>Mass Flows</b>	lb/hr	58290	291833	79024	271100
CO	lb/hr	1.15E-77	0	0	0
CO2	lb/hr	1.33E-52	0	0	0
H2O	lb/hr	1.65E-07	0.56	0.56	0
C1P	lb/hr	4.79E-64	0	0	0
C2P	lb/hr	5.41E-42	0	0	0
C2O	lb/hr	9.54E-48	0	0	0
C3P	lb/hr	1.65E-27	0	0	0
BENZENE	lb/hr	3046	0.0020	0	3046
TOLUENE	lb/hr	2920	0.0117	2.92	2917
C8AROM	lb/hr	2526	18.65	41.0	2504
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	9.60E-13	0	0	0
ISOBU-01	lb/hr	1.86E-16	0	0	0
2-MET-01	lb/hr	0.18	2.73E-27	0.18	0
N-PEN-01	lb/hr	56.5	1.84E-23	56.5	0
N-HEX-01	lb/hr	4765	4.07E-15	4765	0
N-HEP-01	lb/hr	44977	5.28E-08	44977	0
TETRA-01	lb/hr	0	291814	29181	262633

	Units	EXFEED1	EXFEED2	RAFIN	BOTTOMS
<b>Mass Fractions</b>					
CO		1.98E-82	0	0	0
CO2		2.27E-57	0	0	0
H2O		2.84E-12	1.92E-06	7.09E-06	0
C1P		8.22E-69	0	0	0
C2P		9.28E-47	0	0	0
C2O		1.64E-52	0	0	0
C3P		2.84E-32	0	0	0
BENZENE		0.0523	6.91E-09	0	0.0112
TOLUENE		0.0501	4.00E-08	3.69E-05	0.0108
C8AROM		0.0433	6.39E-05	0.00052	0.0092
COAL		0	0	0	0
N-DEC-01		0	0	0	0
N-BUT-01		1.65E-17	0	0	0
ISOBU-01		3.19E-21	0	0	0
2-MET-01		3.02E-06	9.34E-33	2.23E-06	0
N-PEN-01		0.001	6.31E-29	0.0007	0
N-HEX-01		0.082	1.39E-20	0.060	0
N-HEP-01		0.772	1.81E-13	0.569	0
TETRA-01		0	1.000	0.369	0.969

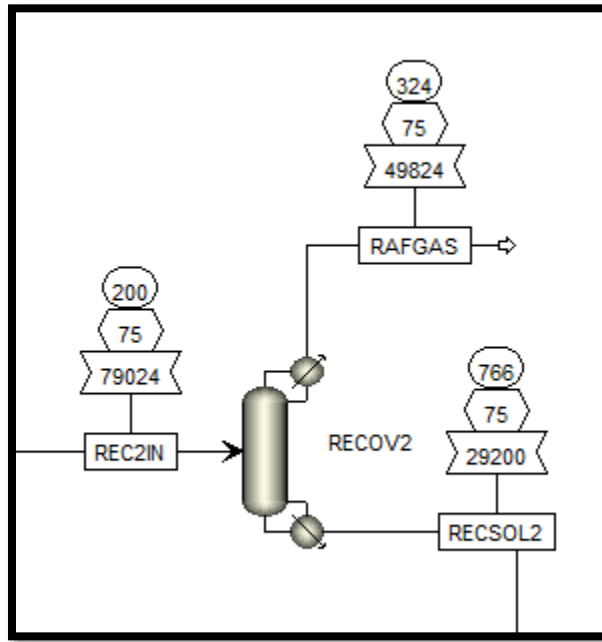
Figure 18 shows the cooler required to cool down the RAFIN stream before entering RECOV2.



**Figure 18. Cooler for RAFIN Stream**

Because RAFIN comes out of EXTRACT at high temperatures, it must first be cooled to effectively model the distillation process for the separation of tetraethylene glycol and the hexane and heptane mixture. This cooler will use cooling water to reduce the temperature of REC2IN to tolerable temperatures.

Figure 19 shows the distillation column used to separate the “raffinate” gas containing heptane and hexane from the tetraethylene glycol solvent.



**Figure 19. Raffinate Recovery Distillation Column**

The separation of heptane and hexane from the tetraethylene glycol solvent is modeled using a distillation column, RECOV2. The solvent is nearly all recovered in RECSOL2, while RAFGAS is essentially all hexane and heptane. The tower will operate with the use of cooling water in the condenser and fuel gas combustion in the reboiler.

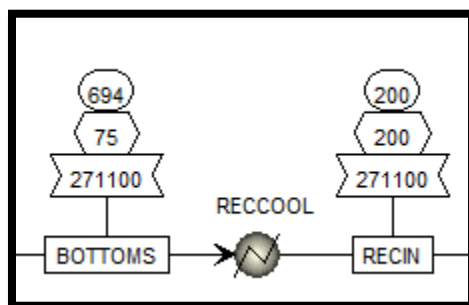
**Table 9. Stream table for Cooler and Raffinate Recovery Distillation Column.**

	<b>Units</b>	<b>RAFIN</b>	<b>REC2IN</b>	<b>RAFGAS</b>	<b>RECSOL2</b>
<b>Description</b>					
<b>From</b>		EXTRACT	REC2COOL	RECOV2	RECOV2
<b>To</b>		REC2COOL	RECOV2		MIX2
<b>Temperature</b>	F	694	200	324	766
<b>Pressure</b>	psia	75	75	75	75
<b>Mass Vapor Fraction</b>		1	0	1	0
<b>Mass Liquid Fraction</b>		0	1	0	1
<b>Mass Solid Fraction</b>		0	0	0	0
<b>Mass Enthalpy</b>	Btu/lb	-918	-1347	-699	-1781
<b>Mass Density</b>	lb/cuft	0.773	39.863	1.027	36.390
<b>Enthalpy Flow</b>	Btu/hr	-72551984	-106475143	-34830615	-52014947
<b>Mass Flows</b>	lb/hr	79024	79024	49824	29200
CO	lb/hr	0	0	0	0
CO2	lb/hr	0	0	0	0
H2O	lb/hr	0.56	0.56	0.56	9.06E-27
C1P	lb/hr	0	0	0	0
C2P	lb/hr	0	0	0	0
C2O	lb/hr	0	0	0	0
C3P	lb/hr	0	0	0	0
BENZENE	lb/hr	0	0	0	0
TOLUENE	lb/hr	2.919786062	2.919786062	2.919785802	2.62E-07
C8AROM	lb/hr	41.0	41.0	22.4	18.6
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	0	0	0	0
ISOBU-01	lb/hr	0	0	0	0
2-MET-01	lb/hr	0.18	0.18	0.18	2.73E-27
N-PEN-01	lb/hr	56.5	56.5	56.5	1.84E-23
N-HEX-01	lb/hr	4765	4765	4765	4.07E-15
N-HEP-01	lb/hr	44977	44977	44977	5.29E-08
TETRA-01	lb/hr	29181	29181	1E-60	29181



	Units	RAFIN	REC2IN	RAFGAS	RECSOL2
<b>Mass Fractions</b>					
H2O		7.09E-06	7.09E-06	1.12E-05	3.10E-31
C1P		0	0	0	0
C2P		0	0	0	0
C2O		0	0	0	0
C3P		0	0	0	0
BENZENE		0	0	0	0
TOLUENE		3.69E-05	3.69E-05	5.86E-05	8.96E-12
C8AROM		0.00052	0.00052	0.00045	0.00064
COAL		0	0	0	0
N-BUT-01		0	0	0	0
ISOBU-01		0	0	0	0
2-MET-01		2.23E-06	2.23E-06	3.54E-06	9.34E-32
N-PEN-01		0.00071	0.00071	0.0011	6.31E-28
N-HEX-01		0.060	0.060	0.096	1.39E-19
N-HEP-01		0.569	0.569	0.903	1.81E-12
TETRA-01		0.369	0.369	2.03E-65	0.999

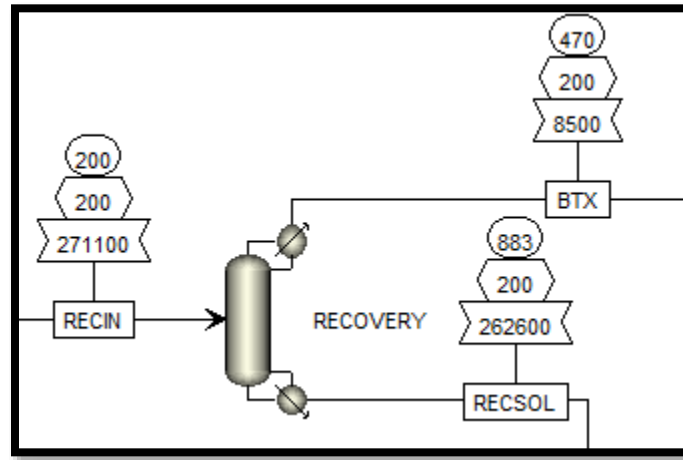
Figure 20 depicts the cooler used to reduce the temperature of the extract from the extraction column.



**Figure 20. Liquid Extract Cooler**

RECCOOL shown in Figure 20 is necessary to cool the BOTTOMS stream from EXTRACT so that it can be effectively distilled for the recovery of the aromatics and the solvent. This cooler will use cooling water to decrease the temperature of RECIN to viable temperatures for the distillation process.

Figure 21 shows the distillation tower used to separate the aromatics from the solvent from the extraction process.



**Figure 21. BTX and Solvent Recovery Distillation Tower**

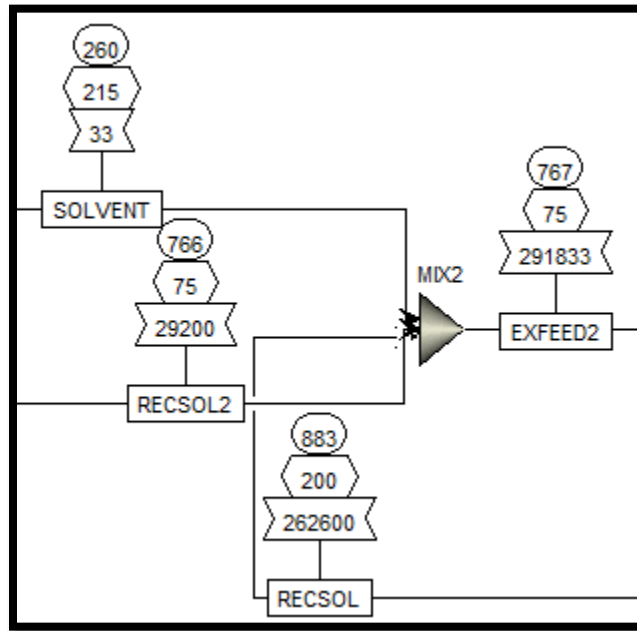
RECOVERY shown in Figure 21 is necessary to recycle the solvent in RECSOL and separate the BTX into an essentially pure stream. The reboiler will use fuel gas combustion and the condenser will use cooling water to operate the tower.

**Table 10. Stream table for Cooler and BTX Recovery Distillation Column.**

	<b>Units</b>	<b>BOTTOMS</b>	<b>RECIN</b>	<b>BTX</b>	<b>RECSOL</b>
<b>Description</b>					
<b>From</b>		EXTRACT	RECCOOL	RECOVERY	RECOVERY
<b>To</b>		RECCOOL	RECOVERY		MIX2
<b>Temperature</b>	F	694	200	470	883
<b>Pressure</b>	psia	75	200	200	200
<b>Mass Vapor Fraction</b>		0.0064	0	1	0
<b>Mass Liquid Fraction</b>		0.994	1	0	1
<b>Mass Solid Fraction</b>		0	0	0	0
<b>Mass Enthalpy</b>	Btu/lb	-1762	-2054	387	-1693
<b>Mass Density</b>	lb/cuft	30.89	50.39	2.26	28.98
<b>Enthalpy Flow</b>	Btu/hr	-477753929	-556928397	3293412	-444617689
<b>Mass Flows</b>	lb/hr	271100	271100	8500	262600
CO	lb/hr	0	0	0	0
CO2	lb/hr	0	0	0	0
H2O	lb/hr	0	0	0	0
C1P	lb/hr	0	0	0	0
C2P	lb/hr	0	0	0	0
C2O	lb/hr	0	0	0	0
C3P	lb/hr	0	0	0	0
BENZENE	lb/hr	3046	3046	3046	0.002
TOLUENE	lb/hr	2917	2917	2917	0.012
C8AROM	lb/hr	2504	2504	2504	0.050
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	0	0	0	0
ISOBU-01	lb/hr	0	0	0	0
2-MET-01	lb/hr	0	0	0	0
N-PEN-01	lb/hr	0	0	0	0
N-HEX-01	lb/hr	0	0	0	0
N-HEP-01	lb/hr	0	0	0	0
TETRA-01	lb/hr	262633	262633	32.67	262600

	Units	BOTTOMS	RECIN	BTX	RECSOL
<b>Mass Fractions</b>					
CO		0	0	0	0
CO2		0	0	0	0
H2O		0	0	0	0
C1P		0	0	0	0
C2P		0	0	0	0
C2O		0	0	0	0
C3P		0	0	0	0
BENZENE		0.0112	0.0112	0.358	7.68E-09
TOLUENE		0.0108	0.0108	0.343	4.45E-08
C8AROM		0.0092	0.0092	0.295	1.91E-07
COAL		0	0	0	0
N-BUT-01		0	0	0	0
ISOBU-01		0	0	0	0
2-MET-01		0	0	0	0
N-PEN-01		0	0	0	0
N-HEX-01		0	0	0	0
N-HEP-01		0	0	0	0
TETRA-01		0.969	0.969	0.00384	0.9999998

Figure 22 presents the mixer used to mix the recycle solvent streams and the make-up solvent.



**Figure 22. Recycle Solvent Mixer**

MIX2 is a mixer that combines the recycle streams RECSOL and RECSOL2 from RECOVERY and RECOV2 and the make-up solvent stream to be fed back to the extraction column. Because of the high recovery of the solvent in RECOVERY and RECOV2, little make-up solvent is necessary in this process.

**Table 11. Stream table for Tetraethylene Glycol Recycle.**

	<b>Units</b>	<b>SOLVENT</b>	<b>RECSOL</b>	<b>RECSOL2</b>	<b>EXFEED2</b>
<b>Description</b>					
<b>From</b>			RECOVERY	RECOV2	MIX2
<b>To</b>		MIX2	MIX2	MIX2	EXTRACT
<b>Temperature</b>	F	260	883	766	767
<b>Pressure</b>	psia	215	200	75	75
<b>Mass Vapor Fraction</b>		0	0	0	0.663
<b>Mass Liquid Fraction</b>		1	1	1	0.337
<b>Mass Solid Fraction</b>		0	0	0	8.76E-10
<b>Mass Enthalpy</b>	Btu/lb	-2166	-1693	-1781	-1702
<b>Mass Density</b>	lb/cuft	49.15	28.98	36.39	1.92
<b>Enthalpy Flow</b>	Btu/hr	-71967	-444617689	-52014947	-496704602
<b>Mass Flows</b>	lb/hr	33.2	262600	29200	291833
CO	lb/hr	0	0	0	0
CO2	lb/hr	0	0	0	0
H2O	lb/hr	0.56	0	9.06E-27	0.56
C1P	lb/hr	0	0	0	0
C2P	lb/hr	0	0	0	0
C2O	lb/hr	0	0	0	0
C3P	lb/hr	0	0	0	0
BENZENE	lb/hr	0	0.002	0	0.002
TOLUENE	lb/hr	0	0.0117	2.62E-07	0.012
C8AROM	lb/hr	0	0.0502	18.60	18.65
COAL	lb/hr	0	0	0	0
N-BUT-01	lb/hr	0	0	0	0
ISOBU-01	lb/hr	0	0	0	0
2-MET-01	lb/hr	0	0	2.73E-27	2.73E-27
N-PEN-01	lb/hr	0	0	1.84E-23	1.84E-23
N-HEX-01	lb/hr	0	0	4.07E-15	4.07E-15
N-HEP-01	lb/hr	0	0	5.29E-08	5.28E-08
TETRA-01	lb/hr	32.7	262600	29181	291814

	<b>Units</b>	<b>SOLVENT</b>	<b>RECSOL</b>	<b>RECSOL2</b>	<b>EXFEED2</b>
<b>Mass Fractions</b>					
CO		0	0	0	0
CO2		0	0	0	0
H2O		0.0169	0	3.10E-31	1.92E-06
C1P		0	0	0	0
C2P		0	0	0	0
C2O		0	0	0	0
C3P		0	0	0	0
C3O		0	0	0	0
C8P		0	0	0	0
BENZENE		0	7.68E-09	0	6.91E-09
TOLUENE		0	4.45E-08	8.96E-12	4.00E-08
C8AROM		0	1.91E-07	0.00064	6.39E-05
COAL		0	0	0	0
N-BUT-01		0	0	0	0
ISOBU-01		0	0	0	0
2-MET-01		0	0	9.34E-32	9.34E-33
N-PEN-01		0	0	6.31E-28	6.31E-29
N-HEX-01		0	0	1.39E-19	1.39E-20
N-HEP-01		0	0	1.81E-12	1.81E-13
TETRA-01		0.9831	1.0000	0.9994	0.9999

**Table 12. System of Control**

<b>Unit Operation</b>	<b>Parameters to Control</b>	<b>Instrumentation</b>	<b>Method of Control</b>
Reactor	Temperature	Temperature Indicator	Flow of char to heating furnace
	Pressure	Pressure Indicator	Recycle Compressor Power
Quench	Temperature	Temperature Indicator	Flow of quench water
Solid Separation Filter	Char Accumulation	Flow Meter	Divert flow to secondary filter during cleaning
Heat Exchanger from Solid Separator	Flow	Flow Meter	Control flow of cooling water through heat exchanger
	Temperature	Temperature Indicator	Control flow of cooling water through heat exchanger
First Flash Unit	Liquid Level	Level Indicator	Control flow of liquid from the unit
Turboexpander Heater	Temperature	Temperature Indicator	Flow of fuel gas to heater
Second Flash Unit	Liquid Level	Level Indicator	Control of liquid from the unit
Recycle Gas Heater	Temperature	Temperature Indicator	Control flow of fuel gas to heater
Compressor	Pressure	Pressure Indicator	Control flow of recycle gas
First Distillation Column Heater	Temperature	Temperature Indicator	Control flow of liquid from Second Flash Unit
First Distillation Column	Temperature	Temperature Indicator	Control reboiler temperature, and flow of cooling water through condenser
	Pressure	Pressure Indicator	Control power to the upstream pump
Extraction Column	Pressure	Pressure Indicator	Control power to the upstream pump
	Temperature	Temperature Indicator	Install a cooler downstream of the solvent recycle mixer
Second Distillation Column Cooler	Temperature	Temperature Indicator	Control flow of liquid from Extractor



<b>Unit Operation</b>	<b>Parameters to Control</b>	<b>Instrumentation</b>	<b>Method of Control</b>
Second Distillation Column	Temperature	Temperature Indicator	Control reboiler temperature, and flow of cooling water through condenser
	Pressure	Pressure Indicator	Control power to the upstream pump
Third Distillation Column Cooler	Temperature	Temperature Indicator	Control flow of cooling water through heat exchanger
Third Distillation Column	Temperature	Temperature Indicator	Control flow of fuel gas to reboiler and flow of cooling water through condenser
	Pressure	Pressure Indicator	Control power to the upstream pump

Table 12 shows the control systems that will need to be installed in order to ensure the plant operates smoothly without major hazards. The biggest area of control is associated with the reactor. With operating conditions at such high temperatures and pressures, it is imperative to install pressure and temperature indicators. The pressure in the system is dependent on the feeds to the system. To control this pressure, the compressor for the recycle gas can be manipulated to alter the pressure of the incoming gas. The incoming solid feed to the reactor comes from a three-stage lock hopper. This hopper will have pressure control implemented in it and can also be used to alter the pressure of the reactor when feeding coal to the process. The temperature of the reactor can be maintained by controlling the feed of the char to the furnace that will be heating the reactor. Another key aspect of control is the quench following the reactor. The quench is necessary to cease the pyrolysis reactions to avoid any undesirable secondary reactions. The amount of water to be used in the quench needs to be controlled to make certain that the temperature of the reactor product stream decreases to acceptable levels based on a temperature indicator following the quench. Another two important aspects of control are the make-up feeds of solvent and natural gas. The feeds to the reactor and extractor must be maintained at the desired rates, so flowmeters must be installed to monitor the feeds and alter the amount of make-up that is fed to the two different mixers. The three different distillation towers require similar control systems. To operate at the conditions necessary to separate the different components effectively, the condensers and reboilers must all be maintained at the operating temperatures. A temperature indicator on each of these could be used in conjunction with flow control of fuel gas to a furnace or flow control of cooling water to maintain the desired temperatures. The other control systems necessary in the process operate similarly to maintain the operating conditions so that the system functions without unnecessary hazards and effectively produces valuable products.

Table 13 introduces the utility requirements of the process.

**Table 13. Utility Requirements.**

<b>Unit Operation</b>	<b>Utility</b>	<b>Amount (MMBTU/hr)</b>	<b>Amount (kW)</b>	<b>Method</b>
Reactor	Heating	1740.93		Char Combustion
Product Cooler	Cooling	-1799.13		Cooling water
Turboexpander Heater	Heating	48.1433		Fuel gas combustion
Recycle Gas Heater	Heating	74.8657		Fuel gas combustion
Recycle Gas Compressor	Electricity		64831.5	Electrical grid power
First Distillation Tower Pre-Heater	Heating	5.35		Fuel gas combustion
First Distillation Tower Condenser	Cooling	-2.33549		Single-Pass Refrigeration
First Distillation Tower Reboiler	Heating	8.3287		Fuel gas combustion
Pump	Electricity		28.8717	Electrical grid power
Raffinate Recovery Distillation Tower Pre-Cooler	Cooling	-33.9232		Cooling water
Raffinate Recovery Distillation Tower Condenser	Cooling	-4.07198		Cooling water
Raffinate Recovery Distillation Tower Reboiler	Heating	23.7016		Fuel gas combustion
BTX Recovery Distillation Tower Pre-Cooler	Cooling	-79.1745		Cooling water
BTX Recovery Distillation Tower Condenser	Cooling	-18.0685		Cooling water
BTX Recovery Distillation Tower Reboiler	Heating	133.673		Fuel gas combustion

The majority of the utility requirements for the process are either heating or cooling of the process streams. All of the cooling required for the process can be accomplished through heat exchangers with a cooling water feed. The only exception to this is the condenser on the first

distillation tower. It operates at 58°F and this is believed to be below the temperature of the available cooling water, so a refrigeration system must be incorporated. This refrigeration will likely be a reasonably simple process as the temperature necessary is not considerably low. The heating requirements for the system can be met with the use of char combustion and combustion of a portion of the purge fuel gas stream. The remaining processes in the system that require a utility are the pump and compressor. Both of these units can be powered with the use of electricity.

In conclusion, the base case provides an adequate solution to processing coal and separating the useful products for the flash pyrolysis of coal in methane within realistic constraints. The base case takes processed ROM coal and reacts it to provide several useful products that can be used in various petrochemical processes. This base case provides essentially pure product streams after processing the reactor outlet stream. Although the operating conditions vary greatly among unit operations, the base case provides effective unit operations that can work well together to minimize utility requirements. With the addition of the turboexpander, useful work can be produced to use around the plant. Additionally, with the recycle stream and the solid char, essentially all the heating requirements can be satisfied. Further work will need to be conducted to effectively model the extractor. All in all, this base case provides the necessary unit operations to accomplish pure product streams with the current specifications and therefore solves our initial goal.

## **Design Alternatives**

The first design alternative for the process is the use of an oil absorption tower as a means of separation. The base case uses a turbo expander to drop the pressure of the TURBFEED stream, allowing the methane to be separated out from the desired products. The oil absorption tower alternative would replace this turbine. The tower would operate with a mixture of alkanes larger than decane as the purity of this mixture is unimportant to the separation. These oils would absorb the hydrocarbons that are larger than ethane. This stream would then go through a distillation column, which would purify our oil and separate out the products. The purified oil would then be recycled back into the absorption tower. This alternative was not used for a variety of reasons. First, it is challenging to model in Aspen+, making data analysis and equipment sizing for the process very difficult. Additionally, it is much more expensive than the turbo expander design in terms of both the cost of equipment and materials, and the operational costs.

The second design alternative utilized a series of four refrigerated distillation columns to separate the methane from the desired products. After modeling and designing this alternative, it was determined that it was a nonviable solution due to the financial burden of the refrigeration process. The refrigeration used over 80% of the plant's total revenue and was the main

contributor to the plant absorbing \$9 million losses annually. Other options were further investigated to find an economically sustainable solution.

Another alternative to consider is the alteration of the methane to coal feed ratio in the reactor. The current reaction operates with a 4:1 methane to dry coal feed ratio. This is problematic when evaluating the cost of separating such a large amount of mass from the desired products. Reduction of the dry coal to methane feed ratio to 1:1 or less would optimize the operational costs utilized to separate the methane from the other products. The issue with reducing the coal to methane ratio is that the product distributions would shift, reducing the BTX and ethylene products created in the reactor.

The last alternative is the separation of BTX into its constituent streams. The current process takes the mixed BTX product stream and sells it as is. Due to the processing required for the purchaser to separate the products, the sale price of the products was lowered to account for the costs the purchaser would be absorbing. This alternative delves into the economic viability of separating the BTX mix stream into a stream of pure benzene, a stream of pure toluene, and a stream of pure xylene compared to selling it as a single mixed stream. Another option within this alternative is to react the benzene and toluene products into more xylene as it has the highest salable value of the three. Both options inside this alternative would increase capital costs as they require additional equipment to complete the processes described and would likely increase operating costs of the plant as well. The key to this alternative is figuring out if the additional equipment and operational costs are outweighed by the additional revenue brought in by the purer, higher value products.

## **Permitting and Environmental Concerns**

The process contains several environmental concerns. The most prominent are the production of phenols in the reactor's water quench and the air emissions produced from pyrolyzing coal. These issues affect the local and global environment if contaminants were to leak outside of the plant boundaries. Both contaminants travel through fluid mediums, so the affected contamination area can quickly grow if not contained or suppressed quickly in the event of a leak or mechanical failure. Both phenol and air emissions are contained safely within the system; however, multiple effluent streams leaving the plant must be treated to decrease the emissions.

Phenol contaminated water is a longstanding issue in industry as it contaminates local water sources at low concentrations. Phenols are highly toxic alone, and they react with organic and inorganic compounds, as well as microorganisms to form phenolic-compounds that may be more toxic than the original contaminants. Phenols are formed when complex organic material is broken down via heat or radiation. They are common precursors used in the chemical processing industry for a multitude of areas such as resins, oil and gas, coal plants, textiles, etc. Due to the high toxicity and expansive use of phenols, a high importance has been placed on total removal of phenols from waste streams leaving plant boundaries. Many techniques have been created for industrial phenol removal which include photocatalytic degradation, ozonation, liquid-liquid

extraction, solid phase extraction, adsorption, and enzyme use. This plant will transport the phenol contaminated water to a nearby wastewater treatment plant that will most likely treat the water using microbes and enzymes to break down the phenols into less reactive constituents. If the wastewater treatment plant becomes nonviable in the future, it would be beneficial to explore treating the water in-house with one of the techniques listed above.

The air emissions from the process occur when coal is broken down by the high heat into smaller compounds. CO<sub>2</sub> leaves the plant in the fuel gas effluent stream that is being sold. No emissions are expected from this stream, but fugitive emissions may occur before it is sold off. Monitoring equipment and routine inspections of the pipes' integrity must be implemented to ensure compliance with federal and state emission laws. In a separate stream, gaseous compounds are vented out of the process in the purge stream to be burned for thermal energy as seen in Figure 1. The plant accounts for this emission stream with the following process operating controls: pyrolyzing the coal in a low oxygen atmosphere to reduce NO<sub>x</sub> formation, burning at high temperatures in a large reactor to reduce incomplete combustion byproducts, and using low sulfur content coal to reduce SO<sub>x</sub> formation. The EPA reports the sulfur content of coal is proportional to SO<sub>x</sub> emissions (EPA citation pg 1.1-7).

Permitting will be a long process and must be started early in the project life to prevent lulls in construction and production. The plant must obtain the permits listed below to comply with federal and state industrial laws:

- Industrial Zoning Permit - Used to obtain the rights to use the land for industrial purposes from the city or state. This permit is the first step in permitting process as it is the foundation for the physical plant.
- Building Permit – Used to ensure the building is structurally sound, safe for occupants, and meets design parameters of local code.
- Hot Work Permit – Safety requirement for builders and contractors using open flames and/or producing heat and sparks. This permit is critical during the building phase to connect piping to various unit operations. This permit will also need to be renewed for repair purposes.
- Confined Space Entry Permit – Used for process safety when workers must enter confined spaces. Moving inside any unit operation for maintenance or repair reasons
- Water Use Permit – Used to justify pulling large quantities of water from geographical regions. Wyoming historically has large drought periods and will require a permit from the local municipality to pull in the needed water.
- Air Emission Permit – Used to monitor compliance with Clean Air Act regulations as the plant is a carbon burning facility.
- Solid Waste Disposal Permit – Used to monitor compliance with Resource Conservation and Recovery Act to ensure proper disposal of solid waste generated at the facility.

The Best Available Control Technology (BACT) data is pulled straight from the EPA's data on external combustion sources for subbituminous coal combustion. Coal burning plants are heavily studied for their emissions, so the EPA has made a comprehensive emission control plan for each plant. To control SO<sub>2</sub> emissions, a dual alkali wet scrubber will be installed for a 90-96% (EPA 1.1-13). To control NO<sub>x</sub>, low NO<sub>x</sub> burners will be installed to decrease NO<sub>x</sub> emissions by 35-

50% (1.1-14). A PC, dry bottom, tangentially fired, sub-bituminous, NSPSg will be used to provide a SO<sub>x</sub> emission factor of 35 lb/ton, a NO<sub>x</sub> emission factor of 7.2 lb/ton, and a CO emission factor of 0.5 lb/ton (EPA 1.1-17). These emission factors all warrant the highest rating of A in the EPA emission scale.

## **Safety and Risk Management**

The system contains several hazardous factors. High temperatures, high pressures, carcinogenic compounds, and combustible materials are all hazardous to the system and to the surroundings. These dangers have been minimized by designing a system that can successfully contain the materials with limited chance of exposure to the environment by conducting a full Hazard and Operability Study (HAZOP). The HAZOP for the process is found in the Appendices as Appendix F.

A significant aspect of the danger of the system is the combustible nature of methane in an atmosphere of oxygen and at high temperatures. The first step to containing methane in an atmosphere devoid of oxygen is passing our influent product stream through a three-stage lock hopper. The three-stage lock hopper is used for the introduction of the coal particles into the reactor. In order to feed the coal into the highly pressurized reactor without introducing oxygen as well, the coal must be pressurized with an inert gas while contained in the hopper. The lock hopper has three stages of inert gas pressurization, which greatly reduces the possibility of allowing any oxygen into the reactor when the coal is fed to the reactor. The small amount of oxygen that does enter the reactor is considered negligible. Another method to reduce the probability of loss of containment and gaseous combustion is the immediate decrease in temperature that follows the reactor. The reactor has a water quench stream which enters and mixes with the hot gases and solid residue. This reduces the temperature of the gaseous products, including the methane, to a point at which the methane will not spontaneously combust if oxygen is increased. The gas is further cooled in a heat exchanger to bring the gas down to ambient temperatures. At this point, the possibility of a leak and combustion is significantly reduced.

Another aspect of hazard that needs to be contained is the possible release of solid coal particles before being fed to the reactor. Prolonged exposure to coal particles in the air can cause severe health effects in the lungs, as well as providing a potential ignition source if the particles should catch fire. To avoid creating an atmosphere containing significant amounts of coal, the coal must be kept within the system. This is accomplished with the use of a self-contained dryer, the three-stage lock hopper, and a filter for the separation of char from the gaseous products. These three operations will each ideally be contained within a shell to prevent any release of solid particles into the surrounding environment.

In addition to the previous examples, a hazard has been identified with respect to controlling levels and flows through various unit operations, and what happens if these levels or flows deviate for an unknown reason. This issue was considered extremely important with devices such as the grinder, lock hopper, reactor, cooler, and flash separator handling too much flow, or having the level inside the device exceed the safe operating limit. The solution was to install both pressure readers and flowmeters to allow early intervention from the operators to adjust or

shutdown the necessary equipment to prevent an issue from occurring. Another solution is to divert flow to another tank or unit operations block in order to prevent an issue from occurring.

High pressure in the system also provides a hazard. The system is at significantly high pressures until reaching the cryogenic expansion step of the process. This hazard is accounted for by appropriately sizing and designing each unit operation for the conditions that it will be exposed to. The materials used for the construction of the process must be capable of withstanding the pressures they are subject to at varying temperatures, and all tanks required in the process are large enough to handle any unknown increase in pressure.

Lastly, there are some adjustments that will be made for personal working at the plant. The tanks will have pressure relief systems, so in the event of an extreme pressure increase they will leak out, rather than increase in pressure and explode. Personal protection equipment will also be required for all personnel working at the plant, and safety checks will be performed at random intervals to ensure that the plant is operating in the safest way possible.

In summary, a significant amount of safety issues with our process involves high temperatures, pressures and dangerous compounds. Safety measures to control flow and level are imperative to preventing failure of the equipment and damage to equipment/operators.

## **Project Economics**

The economics of this Flash Pyrolysis of Coal in Methane process were assessed using *Plant Design and Economics for Chemical Engineers* by Max Peters and Klaus Timmerhaus. The unit operations of the process were sized based upon the inputs and specifications of the Aspen+ flowsheet and were priced based off equipment pricing tables from 2002. The pricing was scaled to May 2018 where it was then updated to January 2020 using cost indices with a 2% increase of the CHE index for the next two years.

The raw material amounts were determined using values from Aspen+ and then costed based on a \$/ton basis for coal and a \$/MMBTU basis for methane. The amount of utilities necessary for the process was determined using the Aspen+ flowsheet. The costs of the utilities were ascertained based upon commonly-cited literature values. The estimated labor cost was determined using assumptions of 8250 operational hours per year and 10 employees per shift.

For the cash flow sheet, the working capital and MACRS5 were calculated based on values given in *Plant Design and Economics for Chemical Engineers* by Peters and Timmerhaus.

All equipment was sized using the parameters listed in Table 14 below. The table lists the equipment ID, the equipment types and description, and the specifications used to price the equipment.



Equipment ID	Equipment Type/Description	Sizing Parameters	Quantity
B1	Rolling Grinder	Capacity=5000 (lb/min)	1
B3	Fluidized Bed Dryer, Carbon Steel	Tower Volume=1.57 (m3)	1
FL-PY	Jacketed Reactor, Stainless Steel, 300 psia	Capacity=0.2 (m3)	1
QUENCH			
SOLSEP	Plate and Frame Separator, Carbon Steel	Filter Area=10 (m2)	2
COOL	Gasketed Plate Exchanger	Heat-Transfer Surface Area=3969 (ft2)	30
FLASH1	Vertical Column, Carbon Steel, 725 psia	Column Height=170 (ft)	1
TURBHEAT	Direct Fired Heater, Carbon Steel Tubes, 500 psia	Heat Duty=802440 (BTU/min)	2
TURB	Axial Gas Turbine	Horsepower=4758.96	10
FLASH2	Vertical Column, Carbon Steel, 725 psia	Column Height=170 (ft)	1
DISTHEAT	Direct Fired Heater, Carbon Steel Tubes, 100 psia	Heat Duty=89166 (BTU/min)	1
DIST	Distillation Column	58 trays, 2 foot tray spacing. Carbon steel sieve trays, 120 foot tower height, 5.6ft diameter	1 tower, 58 trays
COMP	Centrifugal rotary compressor	86940 hp required, 8000 hp per compressor	11
RECHEAT	Direct Fired Heater, Carbon Steel Tubes, 100 psia	Heat Duty=1247631(BTU/min)	187
Split	Piping	40 feet	1
MIX	Motionless Mixer	1 foot diameter	2
PUMP	Cast iron, 150 psi, reciprocating pump	Flowrate=206 gal/min	1
EXTRACT	Priced as a flash column	Diameter of 5.6 ft, height of 120 ft	1
RE2COOL	Carbon-steel, multi tube heat exchanger	Area = 676.741 ft2	1
RECOV2	Distillation Column	Diameter of 5.6 ft, height of 120 ft, 58 trays, carbon steel sieve	1 column, 58 trays
RECCOOL	Carbon-steel, multi tube heat exchanger	Area = 1804.94 ft2	1
RECOVERY	Distillation Column	Diameter of 5.6 ft, height of 120 ft, 38 trays, carbon steel sieve	1 column, 38 trays

**Table 14. ID and description of unit operations via *Peters and Timmerhaus*.**

Table 15 shows the purchase price of each piece of equipment in the process in both 2002 and when updated to 2020:

Unit Operations:	Purchase Price 2002	Purchase Price Jan 2020
B3	\$10,700.00	\$17,000.00
B1	\$700,000.00	\$1,120,000.00
FL-PY	\$11,000.00	\$17,600.00
SOLSEP	\$34,400.00	\$55,000.00
Conveyer for solids from Seperator	\$6,750.00	\$11,000.00
COOL	\$375,000.00	\$600,000.00
FLASH1	\$725,000.00	\$1,160,000.00
TURBHEAT	\$700,000.00	\$1,120,000.00
TURB	\$4,400,000.00	\$7,060,000.00
FLASH2	\$725,000.00	\$1,160,000.00
DIST	\$162,340.00	\$260,000.00
DECHEAT	\$490,000.00	\$790,000.00
DRYER	\$42,000.00	\$67,000.00
COOL2	\$6,000.00	\$9,600.00
DECANTER	\$140,000.00	\$224,000.00
RECHEAT	\$65,500,662.50	\$105,000,000.00
B10	\$3,100.00	\$5,000.00

**Table 15. Unit operation cost breakdown.**

The total capital investment for the plant was determined using the following process. The purchase price of all equipment was found using the method in section “Equipment Costing” above. The prices then needed to be updated from 2002 values to January 2020 values. Since the flash pyrolysis of coal in methane process is a solid-liquid processing plant, the total investment was then scaled up by 503% as per information given in *Plant Design and Economics for Chemical Engineers*. Once this value was determined, a 10% multiplier was added to factor in the price of delivery. The total fixed capital investment of the process was calculated to be \$767,000,000 in 2020.

The flash pyrolysis plant design has several operating costs to consider. Table 16 shows the cost of raw materials for a coal consumption rate of 2.25 billion pounds per year:

Raw Materials:	Amount	Units	Price per unit	Purchase Cost per year
Coal	2250000000	lb per year	\$0.0075000	\$16,875,000

**Table 16. Raw material cost, yearly basis.**

The methane atmosphere for the process is purchased in the form of natural gas since it is composed of over 90% methane. Since the majority of the methane is not consumed during the reaction, the methane from the process is recycled. The recycle is not purely methane, and this is accounted for by implementing a 50% purge stream to keep the contaminant level below acceptable amounts. The purge is then utilized as a fuel source to heat various unit operations throughout the plant. Another significant operational cost of the plant is the cost of utilities. Table 17 contains the utility requirements of the plant as well as the annual cost of these utilities:

Utilities	Amount	Units	Converted	Units	Price per unit	Total Amount per year
Electricity	1886.2	kW	15561150	kwh	0.00692 \$/kwh	\$107,683.16
Steam	33.77	klb/hr	0.03377	Mlb/hr	9 \$/Mlb	\$2,507.42
Natural Gas	3.06E+08	BTU/hr	3.06E+02	MMBTU/hr	\$1.5/MMBTU	\$3,792,245.24
Total Per Year						\$3,902,435.82

**Table 17. Operating cost breakdown, yearly basis.**

The last cost considered for the total operating cost of the plant is labor. Table 18 shows the breakdown of labor costs on an annual basis:

Operating Factor		Workers	Hourly Wage	Yearly Labor Cost
8250	(hr/yr)	10	\$40.00	\$ 5,280,000.00

**Table 18. Labor cost, yearly basis.**

An industry standard of 8250 hours in operation per year was assumed to complete the above labor cost estimation. An assumption of 10 workers per shift was also adopted based on industrial plant advise given by John Myers. The total labor cost includes a multiplier of 1.6 to account for the provision of employee benefits.

The following product streams will be sold to provide a source of revenue to the plant: BTX, fuel gas, and char. Table 19 contains the revenue breakdown for each of the product streams:

Benzene:	\$41,984,600.20
Toluene	\$26,496,019.76
Xylene	\$12,502,235.44
FG	\$147,178,775.53
Char	\$233,553.38
Raffinate	\$69,561,830.00
Total	\$297,957,014.00

**Table 19. Revenue breakdown, yearly basis.**

Table 20 shows the revenue, expenses, and cash flow of the plant over its 20-year operational life on a million-dollar basis.

**Table 20: Cashflow sheet during project life of 20 years, \$1 million basis.**

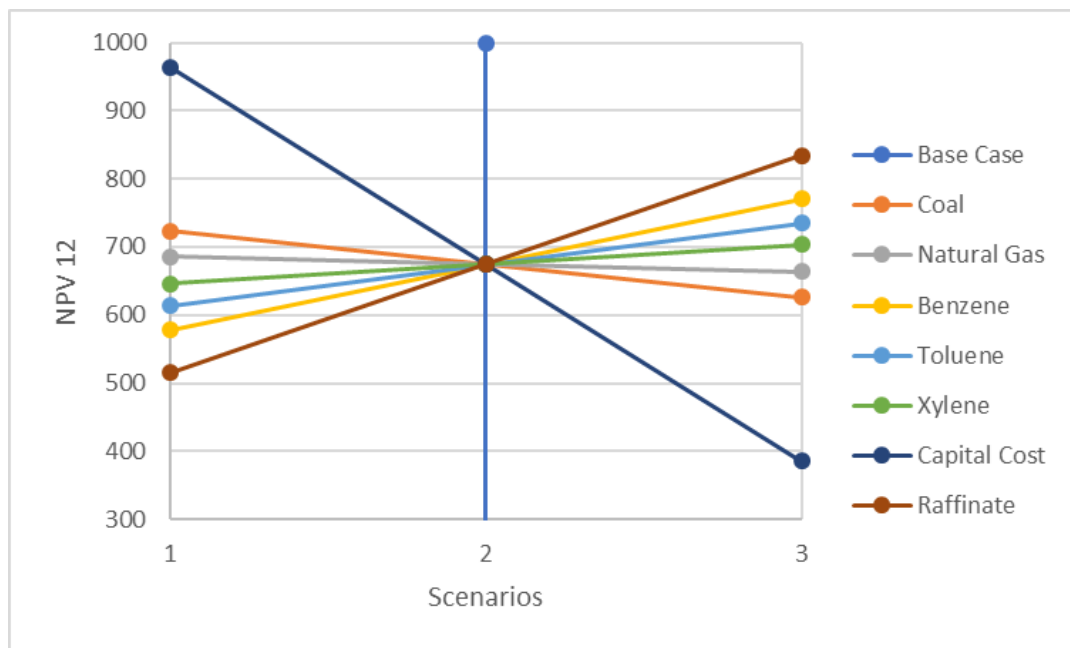
<b>Cash Flow Table</b>	<b>Per Million Basis</b>																					
Tax Rate	21.00%																					
Year (for discounting)(year end)	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	
Total Capital Investment	\$767.8																					
Fixed Capital Investment	\$652.7																					
Working Capital	\$115.2	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	\$0.0	
MACRS5 Factors		\$0.2	\$0.3	\$0.2	\$0.1	\$0.1	\$0.1															
Depr Amount		\$130.5	\$208.8	\$125.3	\$75.2	\$75.2	\$37.6															
Depr Credit		\$27.4	\$43.9	\$26.3	\$15.8	\$15.8	\$7.9															
Nameplate Revenue		\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	
Capacity factor		0.75	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
Revenue		\$223.3	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	\$297.8	
StartUp		\$65.3																				
Variable Costs (scale w/capacity factor)		\$15.6	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	\$20.8	
Fixed Costs		\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	\$5.3	
Total Expenses (including SU)		\$86.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	\$26.1	
Revenue - Expenses (including SU expenses)		\$137.2	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	\$271.7	
Tax Liability on Above Item		\$46.9	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	\$62.5	
Cash Flow	\$883.0	\$117.7	\$253.1	\$235.5	\$225.0	\$225.0	\$217.1	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	\$209.2	
CumCF (PV0)	\$883.0	\$765.3	\$512.2	\$276.7	\$51.7	\$173.3	\$390.4	\$599.6	\$808.8	\$1,018.0	\$1,227.2	\$1,436.4	\$1,645.6	\$1,854.8	\$2,064.0	\$2,273.2	\$2,482.4	\$2,691.6	\$2,900.8	\$3,110.0	\$3,319.2	
DF12	1	0.89286	0.79719	0.7118	0.6355	0.5674	0.5066	0.4523	0.4039	0.36061	0.321973	0.287476	0.256675	0.229174	0.20462	0.182696	0.163122	0.145644	0.13004	0.116107	0.103667	
PV12	\$883.0	\$105.1	\$201.7	\$167.6	\$143.0	\$127.7	\$110.0	\$94.6	\$84.5	\$75.4	\$67.4	\$60.1	\$53.7	\$47.9	\$42.8	\$38.2	\$34.1	\$30.5	\$27.2	\$24.3	\$21.7	
CumPV12	\$883.0	\$777.9	\$576.2	\$408.5	\$265.5	\$137.9	\$27.9	\$66.8	\$151.2	\$226.7	\$294.0	\$354.2	\$407.9	\$455.8	\$498.6	\$536.8	\$571.0	\$601.4	\$628.6	\$652.9	\$674.6	
NPV0	\$3,319.18																					
NPV12	\$674.62																					
IRR	22.88%																					
PBP (approx) (yrs)	6.25																					
MARR	12%																					

Table 21 shows the discounted cash flow analysis of the plant. The Net Present Value (NPV) after 20 years with a discount factor of 12% is approximately \$675 million. The Internal Rate of Return (IRR) is at 22.88%, which is larger than the Minimum Acceptable Rate of Return (MARR) of 12%. The plant has a payback period of roughly 6.25 years. Table 21 displays the discounted cash flow analysis on a per million-dollar basis.

NPV0	\$3,320.10
NPV12	\$675.58
IRR	22.91%
PBB (approx)(yrs)	6.25
MARR	12%

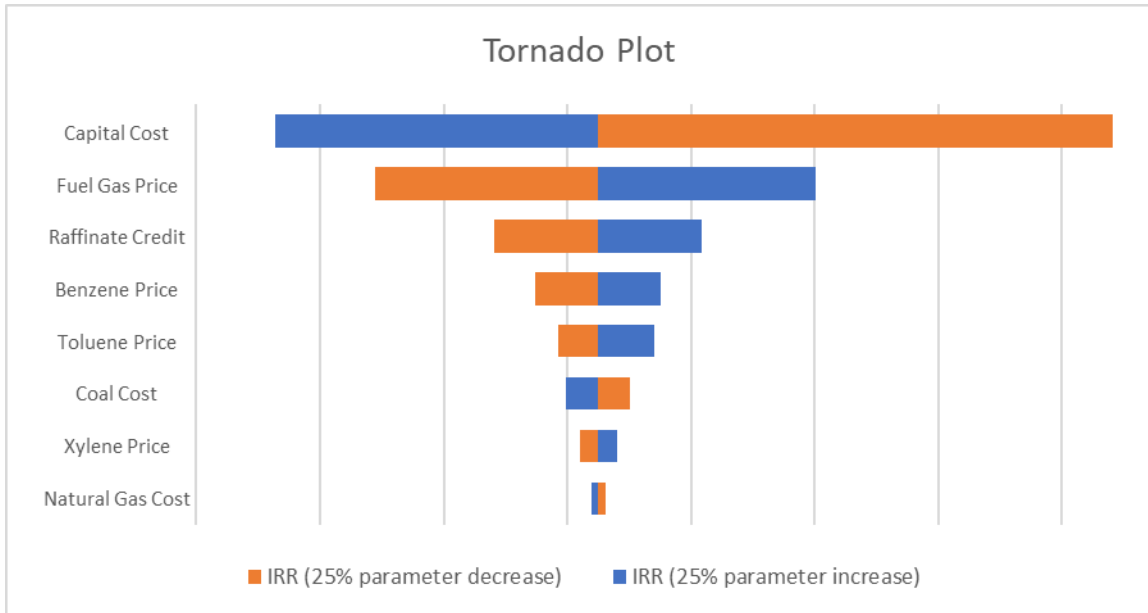
**Table 21. Economic summary.**

A sensitivity analysis was performed on the economics of the chemical plant to estimate the viability of the process with changes to external factors that directly impact the plant. This analysis was completed via a sensitivity plot and a tornado plot. The sensitivity plot contains the analysis of the major economic factors of the process including the sale price of the products, the purchased cost of the feedstocks, and the total capital investment required for the project. The sensitivity analysis was conducted to  $\pm 40\%$  of the base case for each parameter to determine the influence of the parameter on the NPV12 of the process in 20 years.  $\pm 40\%$  was chosen as the range to account for all potential changes to the parameters over the course of the plant's operational life. Figure 23 shows the sensitivity plot for each of the parameters analyzed:



**Figure 23: Sensitivity Plot.**

In Figure 23,  $x=1$  represents the decrease in the parameter by 40% and  $x=3$  represents the increase in the parameter by 40%.  $x=2$  represents the base economic case for the plant. The tornado plot depicts which parameters have the largest impact on the IRR of the plant by varying each of the parameters by  $\pm 25\%$ . Figure 24 shows the tornado plot of seven parameters that could affect the viability of the plant:



**Figure 24. Tornado Plot.**

Figure 24 shows that a change in capital cost and fuel gas price have the most significant impact on the IRR of the process. Benzene and toluene price have a moderate impact on the IRR of the plant when compared to the impact of the capital cost and the fuel gas price. Coal cost, xylene price, and natural gas cost have a relatively small impact on the profitability of the plant and do not require much attention as the process is further developed. The capital cost and the fuel gas price need significant attention as the plant is developed to ensure that the process remains profitable. Some attention should be paid to the benzene and toluene prices as well, but it not as important the top two parameters. None of the parameters when varied by  $\pm 25\%$  caused the IRR to drop below the MARR of 12%.

## Global Impacts

This project has a wide range of global impacts. On the local level, towns in the Powder River Basin area have been facing significant economic challenges due to the decline of the coal industry. This plant could provide an influx of jobs and money to the area, specifically during the construction of the plant. The construction of the plant would bring in approximately 300-400 contractors and their employees to the area for the duration of the plant assembly. Nearby towns

will easily be able to support the additional population since the infrastructural and housing markets in these areas were used to accounting for large population increases when the coal industry was booming. The main benefit of the addition of the construction workers is in the form of tax revenue for the local economy. The contributions they make purchasing fuel, accommodation, groceries, amenities, and other necessities will provide a short term slowing of the economic decline of the area. Unless the coal industry takes a serious turn, this plant will be unable to stop the economic decline of the Powder River Basin area, it will only delay it for a short period of time.

Once the construction of the plant is completed, the economic impact on the local area will decrease dramatically. The plant will employ between 30 and 40 full time employees for operation. The addition of stable jobs will be beneficial for the area, but on such a small scale it is unlikely to have much of an economic impact if any. The area will also lose the economic benefit of having all the construction laborers contributing to the local economy as they move to the next project. The plant will make a small contribution to the local economy through tax revenue, but again it is unlikely to be significant when considering the overall decline of the area. An additional impact on local areas in and around the Powder River Basin is the increase on the demand for coal caused by operating the plant. Over a 20-year period, the plant will process approximately 45 billion pounds of coal from the basin to create high value products. The increased demand could provide much needed economic opportunity for the mining industry and could positively impact local economies to a small extent.

In the global marketplace, the flash pyrolysis plant will take a market share of the petrochemical industry. The plant produces high value products for the industry using an unproven alternative to the standard practices. If the alternative practice proves to be substantially more economical and efficient than the standard practices, the facility would likely be duplicated on a mass scale worldwide. Without that significant improvement over the normal practices, the plant would likely have a very small market share and would have minimal impact on the global economy due to the relatively small scale of the plant as well as a larger desire for purified benzene, toluene, and xylene products rather than a mixed BTX product stream.

## **Conclusions and Recommendations**

The flash pyrolysis of coal in an atmosphere of methane process as designed is an economically viable process. Over the life of the plant, the project makes approximately 674.6 million dollars when operating on a 2.25 billion pounds of coal per year basis. At this feed rate of coal, the reaction yields approximately 70 million pounds of BTX per year and 101 million pounds of fuel gas per year. This makes roughly 81 million dollars and 147 million dollars per year respectively in revenue. The plant remains cashflow positive every year. The payback period was determined to be approximately 6.25 years with an internal rate of return (IRR) of 22.88% which is larger than the minimum acceptable rate of return (MARR) for the plant of 12%. Additional sensitivity



analysis shows that the most significant parameters to consider when deciding to move forward with the plant are the total capital investment and the price of fuel gas. If the total capital investment grows or the price of fuel gas falls significantly, it can prolong the payback period and lower the IRR of a 20-year discounted cash flow analysis significantly. Alternatively, if the total capital investment decreases or the price of fuel gas increases significantly, the payback period will be shortened, and the IRR will grow much larger. Despite the significant impact depicted in Figure 24 of both of these parameters, a change of  $\pm 25\%$  to either parameter will not lower the IRR below the established MARR value of 12% so it would still be recommended that the plant move forward.

Based on the results of this flash pyrolysis plant design, there are numerous recommendations for improving the process to increase both the yield and economic viability. The first recommendation is to investigate the separation of hexane from heptane to see if there is more profitability in the separation and higher sale price of pure hexane rather than the raffinate credit that is received when selling the mixed stream. Another recommendation is to explore the possibility of using any excess char or purge gas as an additional source of revenue by selling it to another plant for use as a fuel. Since such large quantities of material flow through the flash pyrolysis plant, it is likely that not all of the char or purge streams will be required to provide the necessary heating to all of the unit operations. If nearby facilities are willing to pay for the excess to burn for heating in their plants, it could prove a valuable additional revenue stream. A final recommendation is to further investigate the effects of varying the amount of gas that is purged from the system as well as how the impurities from using a natural gas atmosphere impact the product distribution of the reaction. Varying the amount of purge gas could not only impact the amount of potential revenue that could be acquired by selling the excess vapor as fuel, but it could also impact product yields. The foundation of the project was based off Steinberg's research into flash pyrolysis in an atmosphere of methane. Using natural gas that introduces other contaminants into the system has the potential for side reactions to take place that alter the amounts of desired products that are produced.

As it is currently designed, it is recommended that the project move forward with further research. The high value products created via the pyrolysis process are sufficient for the process to become profitable due to the relatively low operational costs of the facility. It is recommended that alternative separation processes and materials are researched more extensively to determine the optimal configuration for the flash pyrolysis plant. If the recommendations and potential alternatives are explored further and prove to improve the plant economics such that the plant becomes even more profitable according to a discounted cash flow analysis, then the given recommendations should be implemented to make the plant even more likely to move forward.

## **Future Work**

The base-line case of the process has had many major improvements from the previous semester. The process never became profitable and had an astronomical yearly cost due to the refrigeration. With the removal of the refrigeration and the ability to remove the fuel gas stream through the use of a turboexpander, the process is currently generating a profit and has a calculatable IRR and payback period. Despite the economic improvements, there are improvements that can be analyzed in future works.

The first is the natural gas composition. Our natural gas has substantial amounts of hexane and heptane within the system. This can be separated into a mixed hexane-heptane stream and sold as “raffinate”. The selling price of raffinate does provide another revenue for our process. However, the sale price of pure hexane and heptane is greater and would bring in a larger profit. No known market for pure heptane is known at this time. If a market for pure heptane is found in the future, it would be economically beneficial to include separation and purification units to sell heptane at 99% purity. Note that there is a big market for hexane but separating hexane from heptane is not economically viable for the price of pure hexane versus the raffinate stream that would not require additional separation.

Another future project would be analytically tracking the mass flow of sulfur from the coal through the process after the pyrolysis. Powder River Basin coal is assumed to have a low sulfur content. However, because of the large feed of coal to the system, sulfur was still be present in the product stream in small amounts. If sulfur compounds were designated in the literature, it would be possible to implement this information into the model. Likely, a scrubber would be necessary to remove sulfur compounds from the products. Future works would include more extensive research into the sulfur-containing compounds from the reactor and the modelling of the removal of these compounds.

Finally, further research needs to be conducted into the presence and amounts of tars and phenol groups in our product stream. At this moment, the Aspen+ model uses molecular composition from the research of Dr. Steinberg’s work which indicates no tars and phenols form at the reactors operating temperature of 1800°F. However, this claim is contradicted in other literature. The Steinberg paper was used as the basis for this project as it provides mass percentages and is the research that our process is scaling up. Due to the contradiction of literature, more research into the reactor product is needed. Consequently, modern research into the mass percentage breakdown of flash pyrolyzed coal at equivalent temperatures is needed to change the literature basis of this process.

To help solve the uncertainties of the process, it is recommended that extra time shall be accounted for in the planning phase of the plant to investigate the future work proposed in this section. The current process is limited to published research available to the public and the University of Wyoming. Conducting research targeted towards completing the future work proposed would aid in increasing the accuracy of the process model and ensuring the economic viability of the plant.

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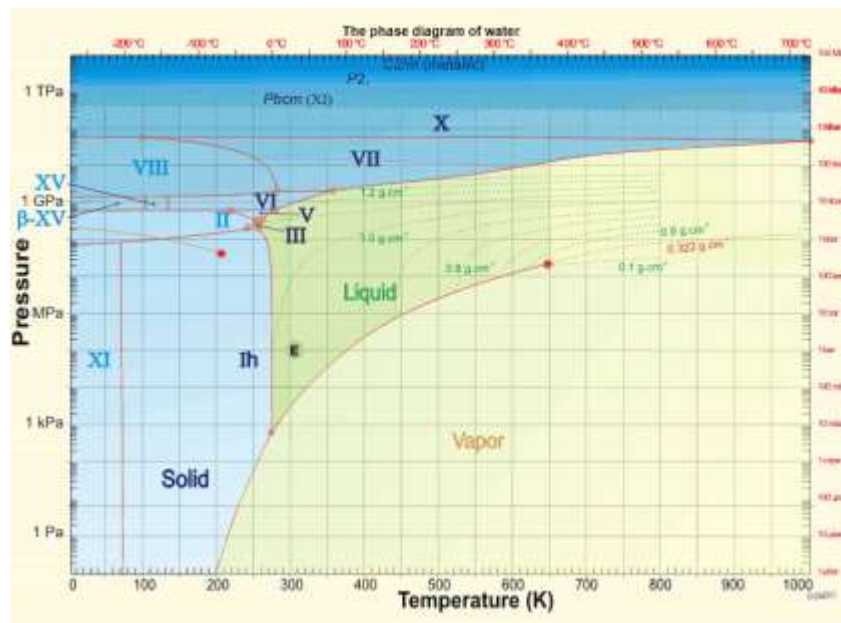
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## Appendices

Appendix A: Three phase diagram of water [IV]



Appendix B: Methane versus Helium for product yield [XXIX]

**TABLE 5**  
Flash Pyrolysis  
of New Mexico Sub-bituminous Coal With Methane

	Run No.				
	683	683	684	692	692
Reactor Temp. (°C.)	900	850	1000	950	1000
Reactor Pressure (psi)	50	50	50	50	50
Coal Feed Rate (lb/hr)	0.99	0.99	1.0	0.9	0.9
Gas Feed Rate (lb/hr)	4.05	4.05	4.05	4.15	4.15
Coal Particle Res. Time (sec.)	1.5	1.5	1.5	1.5	1.5
<b>% Carbon Converted to Product</b>					
C <sub>2</sub> H <sub>4</sub>	10.0	10.2	12.0	12.6	12.7
C <sub>2</sub> H <sub>6</sub>	0	0	0.1	1.1	1.2
Total Gas H.C.	10.0	10.2	12.1	13.7	13.9
BTX	2.9	2.1	9.0	4.2	8.8
Total H.C.	12.9	12.3	21.1	17.9	22.7
CO	6.8	5.7	8.0	4.2	5.4
CO <sub>2</sub>	1.7	1.8	1.7	1.3	1.2
<b>TOTAL</b>	<b>21.4</b>	<b>19.8</b>	<b>30.8</b>	<b>23.4</b>	<b>29.3</b>

Appendix C: Senior Design Product Economics

This excel file contains all of the calculations performed for pricing our units, in addition to the cash flow sheets and excess calculations that were required

#### Appendix D: Final Flow Sheet

This ASPEN file contains the .bkp and .apw file for the process

#### Appendix E: Combined Safety Data Sheets

This pdf file contains all the safety data sheets of the major compounds contained within the plant

#### Appendix F: HAZOP Analysis

This word document contains the full HAZOP analysis for each unit operation within the process