

UNCONVENTIONAL OIL MARKET ASSESSMENT:

EX SITU OIL SHALE

by

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ABSTRACT

This thesis focused on exploring the economic limitations for the development of western oil shale. The analysis was developed by scaling a known process and simulating in ProMax some of the chemical processes implicated in the production of oil shale, obtaining the capital and operating costs to develop these processes and performing an economic evaluation. The final results are a detailed breakdown of the components of the supply cost of syn crude produced.

Two technologies were considered in this project: air-fired combustors and oxy-fired combustors with a CO₂ capture course of action. Additionally, in each of the scenarios, a sensitivity analysis was performed based on the resource quality and the taxation of CO₂ emissions for the air-fired combustion and the price of CO₂ for oxy-fired combustion.

This project revealed that the total capital invested to develop oil shale projects is gargantuan: a total depreciable capital cost of \$3.34 and \$3.39 billion for the air and oxy-fired case, respectively, for a shale quality of 25 gal/ton. It was shown that the geological resource significantly impacts the cost of production. For different shale grades of 20, 25 and 35 gal/ton, the supply cost varied from \$124/bbl, \$112/bbl and \$97/bbl, respectively. Moreover, this analysis showed that the oil shale project profitability is highly dependent on governmental policies. The potential taxation of CO₂ increased the supply cost by 1.75%; the air-base case was \$112/bbl and with CO₂ taxation increased to \$120/bbl.

From these results, it can be concluded that oil shale projects have higher technical, economic and government policy risks which limit their use by industry. For more projects to move forward, these risks must be lowered. It also is clear from the supply cost analysis that royalties are a major component as are taxes and interest charges.

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NOMENCLATURE

Symbol	Definition	Units
C	Costs	\$
CC	Factor determining annual capital charge	1/yr
CF	Annual cash flow	-
D	Pipe diameter	in
d	Depletion	-
E	Effectiveness	-
F	Mass flow rate	lb/hr
H	Head pump	ft
IRR	Internal rate of return	-
k	First order rate constant	h^{-1}
K	Cost of power	\$/kWh
L	Pipe Length	m
LHSV	Liquid hourly space velocity	h^{-1}
NPV	Net present value	\$
n	nth year	-
P	Production capacity	day/yr
PC	Cost of pumping power	\$/kWh
PP	Cost of pipe per diameter per length	\$/in/ft
Q	Volumetric flow rate	gpm

S	Total gross sales	\$
S_{equip}	Equipment Salvage	\$
T	Taxes	-
TF	Toxicity factor	-
W	Weight	Kg
X	Cost of a 2 in schedule 40 carbon steel pipe	\$/ft
x	Mole fraction	-
Y	Hours of operation per year	h/yr
ρ	Density	kg/m ³
μ	Viscosity	N/m
ν	Stoichiometric coefficient	

Subscripts

BM	Bare-module factor
d	Design factor
P	Pressure factor
M	Material factor

CHAPTER 1

INTRODUCTION

Our contemporary society depends intensely on oil, since it supplies about 40% of our total energy demands and more than 99% of the fuel we use for transportation (DOE, 2010). According to the Department of Energy (DOE, 2010), the US and the world may face a crude oil supply deficit in the future. This oil shortfall could be realistically overcome by exploiting unconventional sources such as oil shale, heavy oil and tar sands. In addition, while the US production is expected to decrease, the consumption tends to increase, intensifying the US oil import dependence. The US Energy Information Administration released in July 2010 data showing that only five countries exported more than 1 million barrels per day to the United States and noted that this demand is predicted to increase in the subsequent years (EIA, 2010).

Given that oil shale is one of the alternate sources considered, it is necessary to analyze its features as a potential solution. First, the total oil shale reserves in America are estimated to exceed 2 trillion barrels of oil (Bunger, 2004); while about 1.8 trillion barrels are located in the Green River Formation in western Colorado, southeastern Utah and southern Wyoming (Bartis, 2005). Additionally, oil shale richness or areal density is greater on a per acre basis than other unconventional sources (Bunger, 2004). The areal density can be translated into technical and economic benefits with minimal

environmental impacts. These characteristics of the US oil shale resources call for an intense development to commercialize.

1.1 Overview of Current and Past Oil Shale Production Methods

Oil shale is a rock that contains kerogen, which is a solid hydrocarbon that when heated, yields combustible gases, shale oil and a residue (Baughman, 1978). The first step in producing oil begins with the extraction that can be either *in situ* or *ex situ*, followed by a primary upgrading process, which usually consists of a retort process used to liberate the oil from the solid kerogen in the shale (Strausz, 1978). Afterwards, a secondary upgrading is used with the objective of generating pipeline quality crude oil. Secondary upgrading can take several forms depending upon the oil's characteristics after primary upgrading. Either a coker or hydrotreater is typically used for secondary upgrading (Rana, 2007). Figure 1.1 depicts the steps in the development of oil shale production.

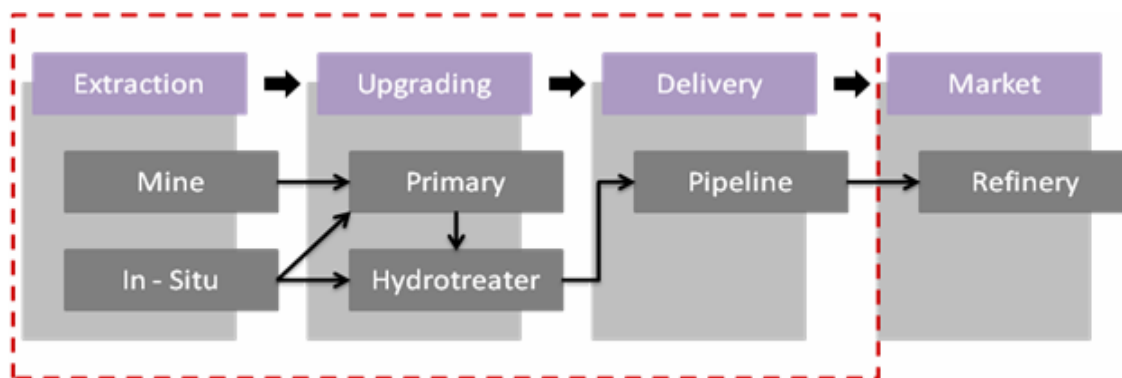


Figure 1.1: Oil Shale Production Methods.

1.1.1 Extraction and Retort Processes

Crude shale oil can be obtained from either *in situ* (underground) or *ex situ* (aboveground) extraction processes. While in an *ex situ* processing, the shale has to be mined and then surface retorted; in the *in situ* process, the deposit is fractured and then retorted underground (Lee, 2000).

1.1.1.1 *Ex situ*

There are two methods to access the oil shale via mining: room and pillar underground mining and surface mining. Underground room and pillar mining recovers about 60% for layers less than a 100 ft thick; whereas surface mining can be used for layers over 1,000 ft and multilayered sources if the resource is relatively close to the surface. Surface mining is subdivided in two types: open pit and strip; open pit can recover up to 90%, but it requires vast areas of terrain (pit~1.5 miles across).

After the extraction process, the oil shale has to be retorted. All surface retorting processes consist of crushing and sizing the shale, heating it (~900°F), followed by cooling and disposal of the spent shale, in addition to sending the hot shale oil to an upgrading process.

1.1.1.2 *In situ*

During the 1970s and 1980s, different *in situ* processes were investigated, involving mainly underground burning of the oil shale to produce heat and thus start the retorting process. However, these methods presented problems in controlling the underground combustion, which were later resolved by a modified *in situ* process. This

modified *in situ* process consisted of mining a portion of the shale which is processed by a surface retort; the remaining shale is broken uniformly by a series of explosions that ignite and burn the underground shale. This modified *in situ* process still requires surface action; therefore, in the early 1980s, researchers considered a new *in situ* recovery process. This new approach consisted of an array of vertical holes, some with a heating element that would heat the oil shale and others for extraction.

1.1.2 Upgrade, Hydrogen Generation and Delivery

Oil shale crude has a very low pour point temperature and high viscosity making transportation difficult and expensive. For that reason, in some cases, it is more economical to have partially refined crude before its transportation; the upgrading site is typically near the retorting site. There are different techniques that can be used to upgrade oil shale such as visbreaking, coking, catalytic hydrogenation and the addition of additives.

Visbreaking involves heating the crude to 900° to 980°F for several minutes. The product is cooled and the gases that developed during heating are eliminated. This process efficiently reduces the oil's pour point and viscosity; however, there is a modest decrease in the nitrogen, sulfur and oxygen content. Alternatively, the coking process starts by heating the oil to the same temperature as visbreaking; followed by charging the heated oil into a vessel, where thermal decomposition occurs. Inside the vessel, the coke is allowed to fill two-thirds of the drum before the feed is switched into another one.

Catalytic hydrogenation is the most expensive process. It produces the highest quality products, meaning low nitrogen, sulfur, oxygen and olefinic content. Catalytic

hydrogenation reacts the shale oil with hydrogen in presence of a catalyst. Hydrotreating opens ring structures and shortens the lengths of the hydrocarbon molecules in the crude oil and also plays an important role in removing some of the sulfur as H_2S , nitrogen as ammonia and heavy metals.

Additionally, since hydrogen is needed for the catalytic hydrogenation process, hydrogen generation is required. A typical hydrogen plant uses natural gas, oxygen and water as feeds to produce H_2 in three steps. The key step for producing hydrogen comes from the reaction between methane and water. However, this reaction is endothermic and requires a large amount of heat. The primary source of that heat, which also adds an additional amount of H_2 , comes from the partial combustion of natural gas in a gasifier. Finally, CO in the syn gas from both the steam reformer and gasifier can be combined with water in a water-gas shift reaction to produce more hydrogen.

1.1.3 Economic Analysis Methods

With the annual production rate and the price of synthetic crude oil established, the total annual sales can be easily determined as the product of these two values. Much of the effort of this chapter then shifts to the calculation of supply costs. Supply costs are in two broad categories and consist of capital and operating costs for a given year. Capital costs are the percentage of the total direct capital costs that are depreciable in a given year. Operating costs come in two broad categories: fixed and variable. They include land, working capital, utilities, labor, maintenance, taxes and royalties. Many of these costs are developed based upon the total depreciable capital for the processing

plant. The total depreciable capital is determined by summing up the cost of each piece of equipment needed for the process as well as any installation expenses.

1.1.4 Equipment Costing Methods

Supply costs will be developed for the various scenarios using industrial standard methods for the estimation of capital and operating costs for each year over the life of the project. Standard accounting methods are used to establish discounted cash flow predictions for the project, allowing various measures of profitability to be established. Operating costs are determined by accounting for 1) the direct manufacturing costs, including feed stocks, utilities including electricity, water (steam, cooling and process), refrigeration, fuels, solid waste treatment, waste water treatment and air pollution abatement as well as labor and maintenance, 2) operating overhead, and 3) fixed costs, including property taxes and insurance, depreciation, as well as general expenses, including selling (or transfer) expenses, research (direct or allocated) expenses, administrative expenses and management incentives. Surface mining costs are estimated from methods used in civil engineering for large excavations. We will use a mixture of capital costing methods for this project including the following:

a) Hill's Method (Hill, 1956)

To produce an estimate, only two things are needed: a production rate and a flow sheet showing the major pieces of equipment, including gas compressors, reactors and separation equipment. Heat exchangers and pumps are not considered in making the estimate. The estimate uses the Marshall Stevens Process Industry Average Cost Index to account for inflation in this industry. Different types of processes, e.g. fluid vs. solids

handling, have different cost estimating factors. Additional factors to account for site preparation, services facilities, utility plants and related facilities can be added. The estimate is accurate to approximately $\pm 50\%$ and is particularly useful for low-pressure petrochemical plants.

b) Lang's Method (Peters, 1968)

This method requires a process design, complete with a mass and energy balance and equipment sizing. The estimate uses overall factors that multiply estimates of the delivered cost of all the process equipment, including heat exchangers, pumps, gas compressors, reactors and separation equipment. Important factors account for the effects on unit cost of construction materials, operating pressure and delivery costs of the equipment. The estimate uses the Marshall Stevens Process Industry Average Cost Index to account for inflation in this industry. Different types of processes, e.g. fluid vs. solids handling, have different cost estimating factors. Using various Lang factors, either the total permanent investment (fixed capital investment) or the total capital investment (including working capital at 17.6% of total permanent investment) can be determined. The estimate is accurate to approximately $\pm 35\%$.

c) Guthrie's Method (Guthrie, 1974)

The method requires an optimal process design with mass and energy balance, equipment sizing, selection of construction materials and a process control configuration. To apply the Guthrie method, f.o.b purchase cost of each piece of equipment is estimated as is the case with the Lang method. Instead of using an overall factor to account for equipment installation and other capital costs, individual factors for each type of equipment are used. This allows the construction materials to be different for a reactor or

separation unit and the platforms and ladders required to access it, for example. To the summation of installed equipment costs, the components of total permanent investment, including contingency and contractor fees, site development costs, building costs and offsite facility costs are added. The total permanent investment cost is added to the working capital to determine the total capital investment. The estimate uses the Chemical Engineering Cost Index to account for inflation by equipment type in this industry. The estimate is accurate to approximately $\pm 20\%$.

A similar *ex situ* oil shale case was done in the 1980s by Weiss at MIT's Energy Laboratory. We cannot improve on that processing route but will modify it to a new site and today's standards. The capital costs have been updated for a new production rate and a 2010 purchase date using Hill's method and the operating costs have been updated to modern unit operation costs. In all other cases, the capital costs have been estimated by the Guthrie method where possible or the Lang method where not. The annualized costs of the capital investment are determined over the life of the plant, giving annualized capital expenses which are added to the annual operating costs for the plant to determine the annual cost for producing the annual production of the plant. The annual cost divided by the annual production rate of the plant gives the supply cost for that year. Making assumptions about the sales price for the crude oil to the refinery and its price sensitivity, the pretax profit from the production and upgrading operations developed for this scenario will be determined as well as the depreciation, depletion and income taxes for these operations. Finally, various rigorous profitability measures such as annual cash flow, annual net present value and investor's rate of return will be determined.

1.2. Obstacles to Development

Oil shale development is constrained by various factors such as the economics and the environmental impact involved in its production.

An oil shale facility can be very costly, meaning expensive oil. Although the price of oil shale is expected to be competitive now and in the future, it is still a risky investment. This investment consists not only of the mining, retorting and upgrading design and development aspects, but also requires a supporting infrastructure such as roads, pipelines, power lines, waste treatment and pollution control facilities. According to a government supported operation in Colorado, it required an investment of \$1.2 billion (2005 dollars) and a production cost of approximately \$ 100 per barrel (2005 dollars).

Waste disposal is one limitation to oil shale development. Retorting produces large quantities of waste rock which undergo a 10% volume increase during the process; these rocks generate a disposal problem (Yen, 1979). Allain (Allain, 1980) reported that 10^{12} Btu of oil produced generates over 350,000 tons of spent shale. On addition, the spent shale still contains significant quantities of oil which require treatment before disposal. Air pollution also has to be considered as another constraint. The production of oil generates major pollutants such as CO, NO_x and SO₂, as well as particulates generated from crushing and blasting oil shale rocks (Allain, 1980). Another environmental limitation is dictated by the oil shale's location which has a limited water supply since its sources are mainly concentrated in semi-arid areas. Water consumption and water disposal are major problems. These issues create the necessity for a new contingent infrastructure that has to be considered such as reservoirs, solid waste

treatment plants and pipelines. Moreover, the surface area required for mining and retorting can create land damage which influences natural flora and fauna, as well as the natural aesthetic beauty of the landscape (Allain, 1980).

Although the aforementioned issues affect oil shale development, the central economic problem is the fact that it is only about 10-15% of the mass is recoverable as marketable energy and the remaining 85-90% incurs a considerable expense just to process and dispose of it in an environmentally acceptable manner. By contrast with conventional fossil fuels, essentially 70-90% of recovered product ((e.g. 70-90% of coal, up to 100% (ex water and sulfur) of natural gas and 100% (ex water) of oil)) consists of usable energy, i.e. burnable. Conversely, large volumes of shale must be mined, handled, processed and disposed of in order to recover a relatively small amount of shale oil by traditional methods of surface retorting; all of that is expensive.

In some locations, a second key problem exists: heavy burdens imposed by the particular location – Utah's Uinta Basin. The terrain is difficult, making construction expensive. Water supplies are limited; their use for energy purposes has provoked serious social and institutional debate for over 30 years. Population is sparse; the infrastructure does not exist to provide and support the people needed to build and operate an oil shale industry. Environmental restrictions may limit the size of the industry or require more extensive (and expensive) emission controls for air, water and solid wastes.

One technical approach to the lean-ore problem is *in situ* extraction. By leaving all or most of the rock in the ground and processing it there, materials handling problems are significantly reduced. Several methods of *in situ* recovery have been proposed and

researched. Although technical feasibility has been demonstrated oil can be produced, economic feasibility has not been demonstrated to date and the future for *in situ* recovery is not clear.

1.3. Goal of the Project

The purpose of this project is to examine the limiting factors to oil shale development and determine the commercial viability with a supply cost analysis. To complete this study, an engineering cost estimate was performed, an assessment of market conditions under which processes breaks even as well as a sensitivity of processes to price volatility and resource quality.

CHAPTER 2

PROCESS DESCRIPTION

2.1. Scenario Specifications

This project studied oil shale production at a scale of 50,000 barrels a day. The location of this resource is the OSEC property near Bonanza, UT, as shown in Figure 2.1. This resource is estimated to have a quality ranging from 25 to 35 gallons per ton of oil shale (Baughman, 1978).

The technology used assumed a room-and-pillar mining process with one-bench and a 60ft thick seam at a depth ranging from 600 to 860 feet and a TOSCO II retort. The hydrotreater was specified to be a trickle-bed reactor with a commercial NiMo/Al₂O₃ catalyst, while the hydrogen plant was based on a steam reformer/gas shift reaction. The pipeline is assumed to run in a straight line from the mine location to Vernal and then to North Salt Lake, UT., with an approximate distance of 379.6 km.

The oil shale scenario was divided in two cases, one assuming oxy-fired combustion with a CO₂ sequestration process. This process mainly consisted of a compression/cooling process to produce a pipeline quality CO₂ product. The other case assumed a regular air-fired burner with stack emissions.

In the air case, air was assumed to be 20% oxygen, 79% nitrogen and 1% argon on a mole basis, while in the oxy-fired case, it was assumed to be pure oxygen.



Figure 2.1: Bonanza and Mine location

In each case, a sensitivity analysis of the shale resource grade is performed taking as a basis a 25 gal/ton source and varying the grade down to 20 gal/ton and up to 35 gal/ton.

2.2. Characteristics of Utah Oil Shale

Typical characteristics of Uinta Basin oil shale are given in Table 2.1. The average Fischer assay is 25 gal/ton for the Green River deposit in this area but a considerable fraction of the deposit has a higher assay of 35 gal/ton or higher (Baughman, 1978).

Table 2.1: Characteristics of Utah Oil Shale (Weiss, 1982)

Oil Content (Fischer assay)	35 gal/ton
Average Mineral Composition:	
<u>Mineral</u>	<u>Composition wt%</u>
Dolomite	32
Calcite	16
Quartz	15
Illite	19
Albite	10
K feldspar	6
Pyrite	1
Analcime	1
Probable Composition of Organic Matter	
<u>Component</u>	<u>Composition wt%</u>
Carbon	80.52
Hydrogen	10.30
Nitrogen	2.39
Sulfur	1.04
Oxygen	5.75
H/C atomic ratio	1.54
Liberation Particle Size:	
	90% less than 20 microns; mass median 5 microns
Moisture	1%
API density	20-26

The sample presented in Table 2.1 has an assay of 35 gal/ton, a carbon content of ~80% by weight and a hydrogen to carbon atomic ratio of 1.54, and with the mineral content being primarily carbonate minerals, dolomite and calcite. Figure 2.2 shows an isopach and overburden thickness for a continuous interval averaging 25 gal/ton.

2.3. Process Overview

In this scenario, we will focus on *ex situ* extraction involving mining and surface retort technologies to extract the oil from the oil shale. The location of this resource is the OSEC property near Bonanza, UT, as shown in Figure 2.1. The Mohogany zone

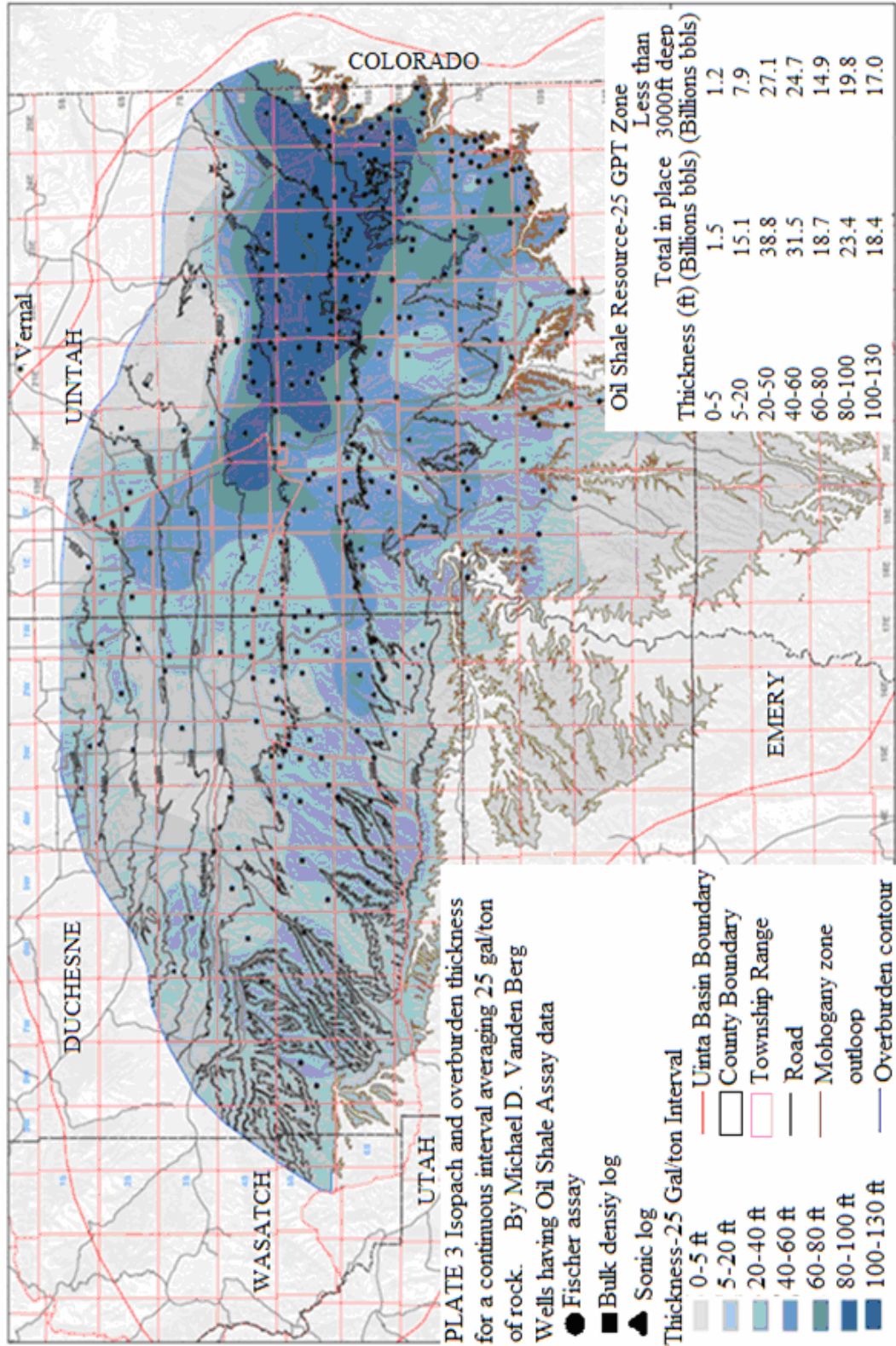


Figure 2.2: Basin-wide Evaluation of the Uppermost Green River Formation's Oil-Shale Resource, Uinta Basin, Utah and Colorado (VandenBerg, 2008)

varies considerably in this area but is approximately 1,000 ft deep, suggesting that underground mining is possible. Ore beneficiation using fine grinding and froth flotation before retorting was studied by (Weiss, 1982) and was not found to be an economic improvement over direct retorting. This was due to the high capital and energy costs for grinding for the flotation step as well as the added uncertainty of the process. Grinding technology has not significantly improved since the time of the Weiss report so ore beneficiation has not been considered in this assessment (Weiss, 1982). Supercritical extraction may also be used for beneficiation but this technology is even more highly uncertain than that of froth flotation. However, it may play a role in *in situ* methods.

Underground mining for oil shale starts between 500 and 2,000 ft down in an underground mine. The oil shale is blasted from the mine's wall and transported to the surface where a comminution circuit grinds it down to less than 0.5 in and it is placed in covered storage. The ground shale is moved by belt conveyor to the retort. Any one of a number of retort technologies (Tosco II, Lurgi, Paraho direct (licensed to Petrobras), Union B) could be used, but for this case, the Tosco II retort was used since a large amount of commercial experience was obtained in the 1980s with Exxon's Colony project.

Once retorted, the raw shale oil is stored in tanks under hot conditions. The raw shale oil is then moved to the hydrotreater where hydrogen is added and sulfur, nitrogen and heavy metals are removed. A schematic of this extraction and upgrading process is given in Figure 2.3. Each of the unit operations is discussed in the sections that follow. This discussion first identifies the individual pieces of major equipment needed and

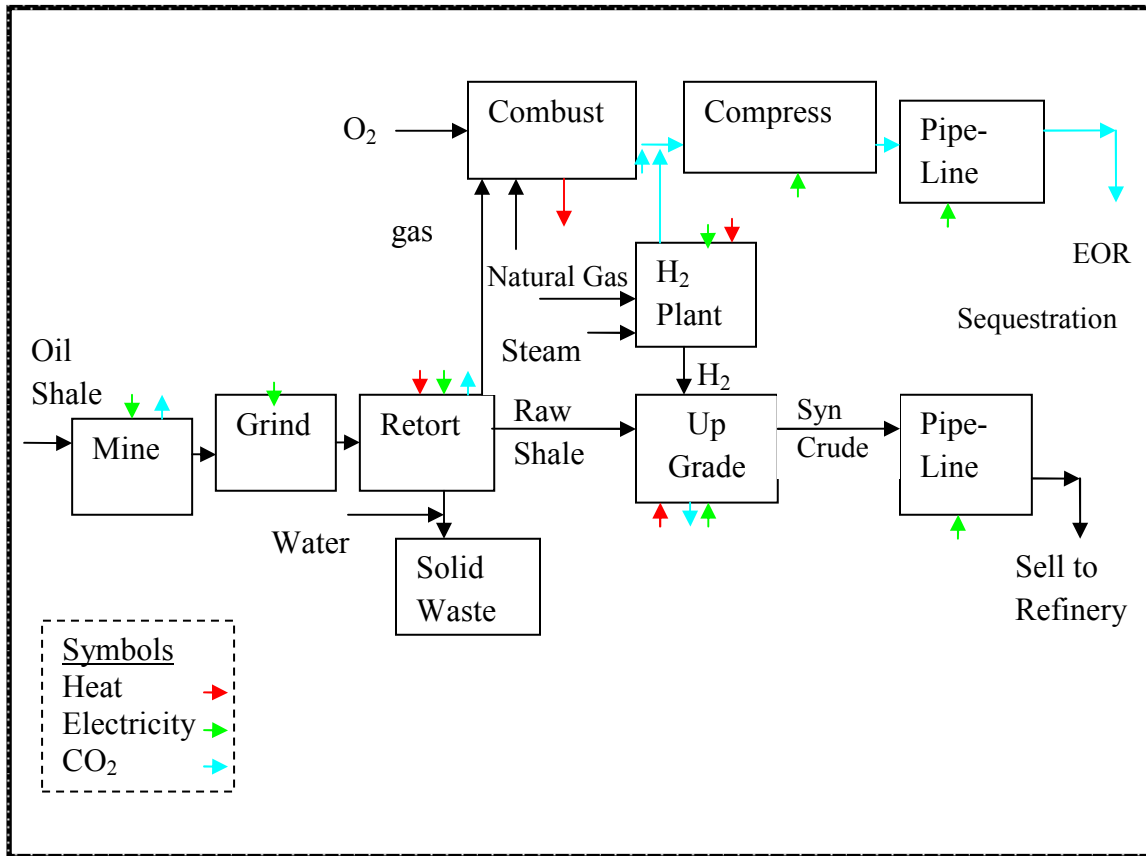


Figure 2.3: *Ex Situ* Oil Shale Extraction Process Overview Using Oxy-fired Combustion

then proceeds to estimate the capital and operating costs for the units to determine the supply costs for the given production rate of synthetic crude oil.

2.3.1 Mining

The ore is to be mined by the room and pillar method as described in Exxon Colony's environmental documentation (Weiss, 1982). The mining section includes in-mine haulage, primary cone crushing, the required surface truck fleet and coarse shale storage.

The quantity of rock that must be mined each day at 25 gal/ton oil shale grade is 85,512 ton/day to yield 50,000 bbl/day.

2.3.2 Comminution and Solids Handling

Oil shale particles are separated by density since kerogen density averages about 1.07 while the density of the minerals averages 2.7 (Weiss, 1982). To perform this separation, it is necessary to crush and blast oil shale rocks followed by comminution. The additional comminution includes secondary crushing (to 0.5 in), covered storage of crushed shale and a linking belt conveyor system from the grinding units to the storage system. Impact crushers are used for secondary crushing.

2.3.3 Pyrolysis

The process design of the pyrolysis section was based chiefly on the environmental documentation from the Exxon Colony Project (Weiss, 1982). The flow sheet is shown in Figure 2.4. The plant has six parallel trains. The design criteria are listed in Table 2.2. The raw shale from the second stage crusher is preheated with flue gases from the ball heater and fed into the retort together with steam and hot ceramic balls that act as a heat transfer medium. The retort includes a rotating inclined drum in which the shale and balls are intimately mixed before they pass into the accumulator. Overhead vapors include hydrocarbons, carbon monoxide and dioxide, ammonia, hydrogen sulfide, water and hydrogen. They are quenched with cooling water and separated into gas, naphtha, gas oil, bottoms oil and foul water in a fractionator. The

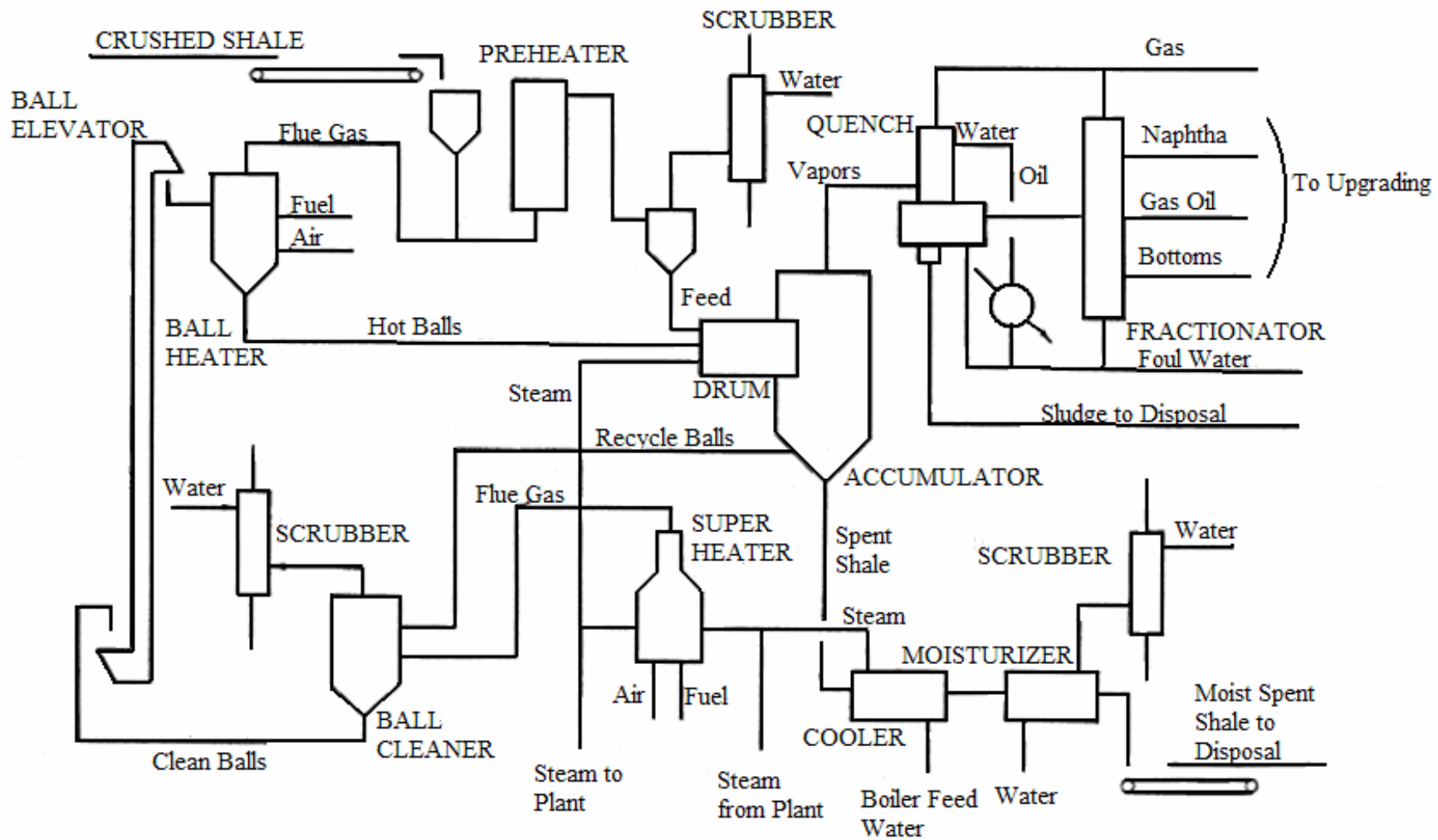


Figure 2.4: Process Flow Diagram for the Pyrolysis Section (Weiss, 1982)

Table 2.2: Design Criteria for Pyrolysis, (Weiss, 1982)

Design Criteria	
A. Pyrolysis and Fractionation	
1. Material Balance	
Raw shale, k tons/day	66
Shale oil, recovery, %	90
Moisture, %, raw shale	1.4
Moisture, %, spent shale	14
Moisture, %, pyrolysis vapor	1.2
Pyrolysis vapors, lbs/lb shale	0.182
Fractionation products, wt%	
Gas	25.1
Naphtha	10.4
Gas Oil	45.6
Bottoms oil	18.9
Balls, lbm/lbm shale	1.5
2. Temperatures °F	
Shale feed after preheater	500
Shale feed to retort	900
Balls to retort	1300
Flue gas after preheater	130
Spent shale after cooler	300
Spent shale after moisturizer	200

naphtha separation together with processing of the other streams is part of the upgrading section.

The spent shale is separated from the balls in a rotating trommel screen at the bottom of the accumulator and is discharged through a cooler (waste heat recover) boiler to a moisturizer.

The moist spent shale is then taken by conveyor to the waste disposal area. The balls are recycled to the retort drum via a cleaner and heater. In the cleaner, dust is removed from the balls using the flue gases from a steam super heater. Steam facilities are not fully shown in Figure 2.4 because they are integrated with the steam generator for the entire plant. The spent shale contains all the original raw shale with a few percent of unrecoverable kerogen or its nonvolatile organic derivatives. The waste effluents and corresponding pollution control equipment are summarized in Table 2.3. The data are based on the environmental documentation from Weiss (Weiss, 1982).

Dust from the conveyor belts is a relatively small pollution source. Gas and liquid effluents from the pyrolysis step originate primarily from the kerogen. Dust effluents from the pyrolysis originate primarily from the oil shale.

The tailings (and associated water) are expected to liberate soluble salts, trace elements but not residual organic material, e.g. (Weiss, 1982). For that reason, the tailings pit will be top and bottom lined.

2.3.4 Secondary Upgrading

For oil shale from the Green River Formation in Utah, the raw shale oil is light enough (fitting into the right side of the High conversion box in Figure 2.5 to be

Table 2.3: Pollution Control

Section and Equipment or Facility	Material Controlled	Type of Control	Flow Rate Unit
Mining			
Mine stockpile	Shale dust	Water sprays	-- *
Primary Crusher	Air + Shale dust	Fabric filters	62 k acfm
Secondary Crusher	Air + Shale dust	Fabric filters	70 k acfm
Storage Building	Air + Shale dust	Fabric filters	36 k acfm
Waste disposal	Spent shale or tailing, etc.	Landfill	55 k tons/day
Conveyors	Shale dust	Foam sprays	--
Pyrolysis			
Preheat system	Air+feed dust, Hydrocarbons	Scrubbers, Thermal oxidizers	210 k acfm 350 k acfm
Ball cleaners	Flue gas + feed dust	Scrubbers	44 k acfm
Moisturizers	Air + spent shale	Scrubbers	44 k acfm
Conveyors	Spent shale or residue dust	Foam sprays	--

*Dashes (--) indicate flow rates that vary widely or do not significantly affect control equipment selection and sizing.

directly hydrotreated, avoiding any additional processing).

After the oil shale is extracted, processed and sent into the fractionators, all blend streams (the naphtha, gas oil and the bottoms oil) are sent to three different hydrotreaters for upgrading. The gases are sent to a burner for heat generation. The combination of the nonrefined blends has the properties of what we call raw oil, while the refined oil's features are the upgraded target. These properties are shown in Table 2.4.

The upgrading process described in Figure 2.6 begins in the feed pumps. Here the naphtha, gas oil and bottoms are pumped from standard temperature and pressure (STP, meaning 25°C and 1 atm) to 8.8MPa, followed by a preheating step in a heat exchanger

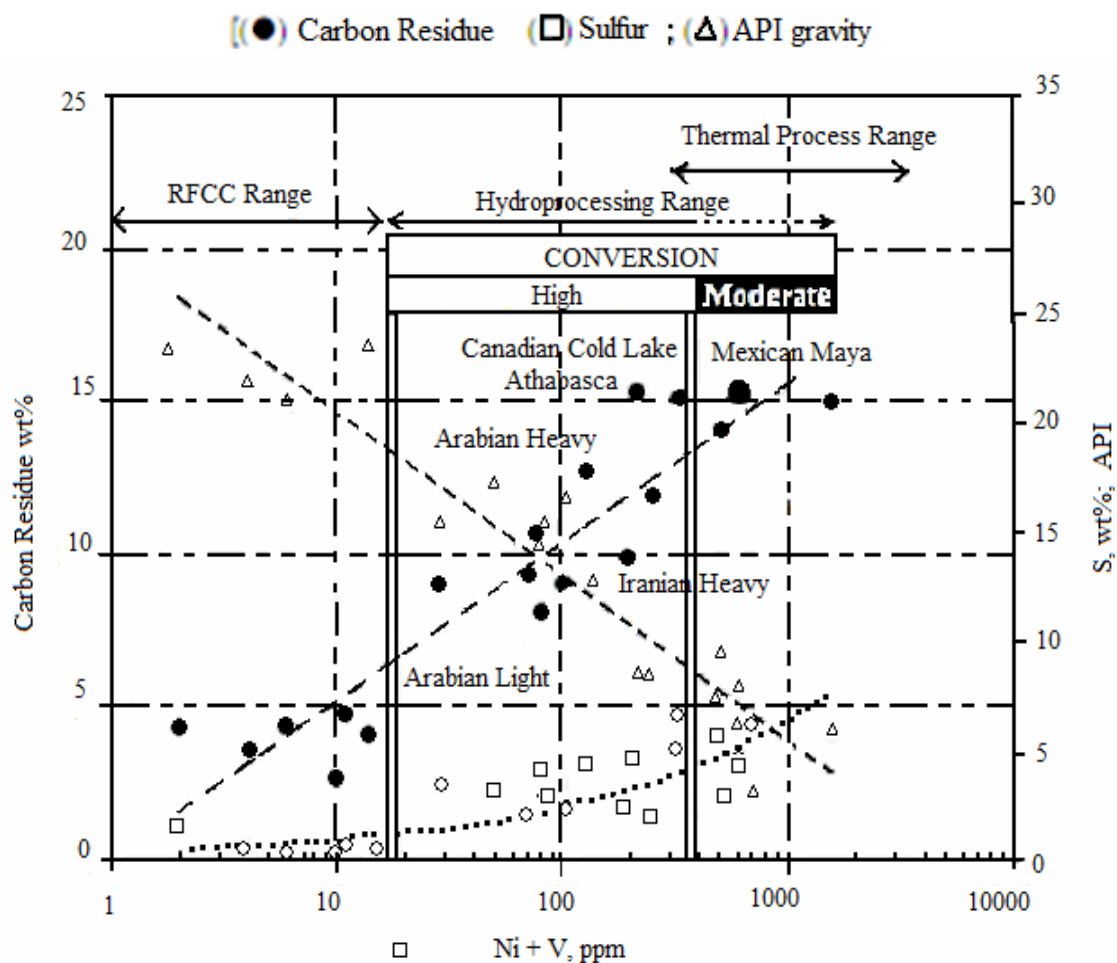


Figure 2.5: Heavy Oil Upgrading Choices as a Function of 343°C Residue Properties.
(Rana, 2007)

Table 2.4: Raw and Upgraded Oil Characteristics, (Utah Heavy Oil Program INSCC, University of Utah, 2007)

	Raw shale oil	Upgraded shale oil
API	20-26	38
Sulfur, wt%	0.7	0.01
Nitrogen, wt %	1.9	0.1
Pour point °F	70-90	0
Solids, wt %	1-2	—
Distillate, vol %		
104-800 °F	54	73
800 °F+	45	26
1000 °F+	7	2

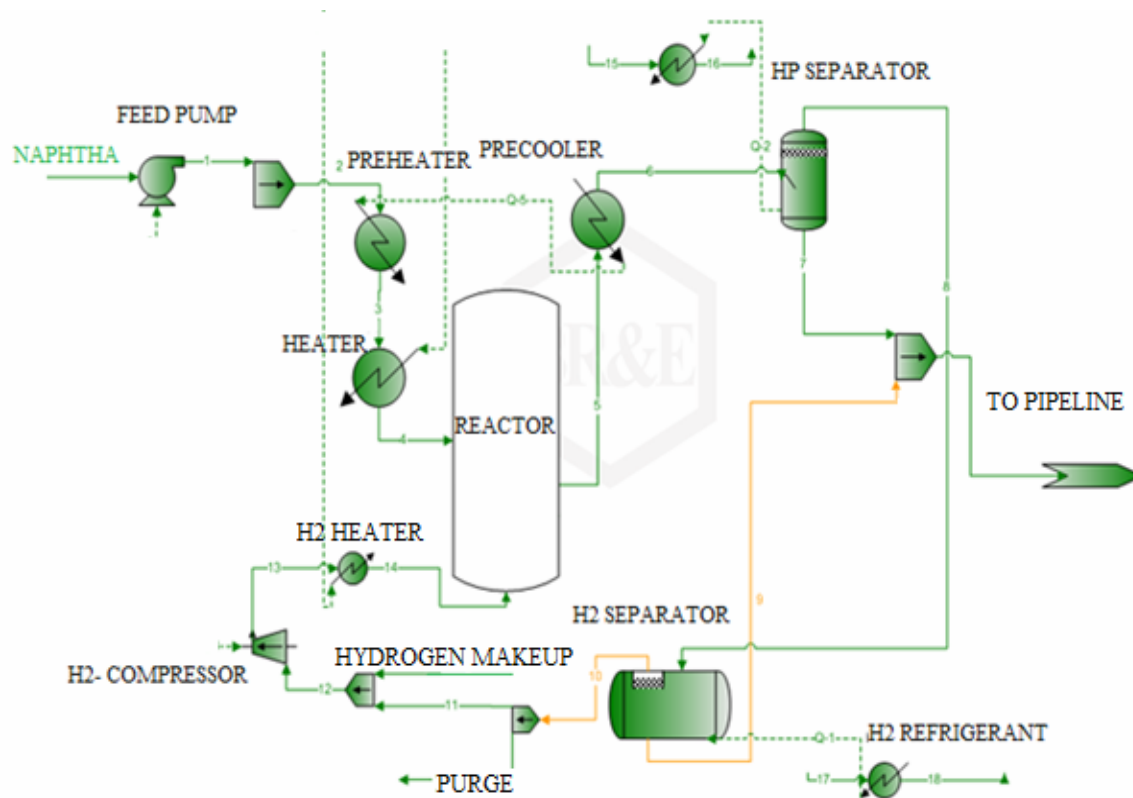


Figure 2.6: Process Flow Diagram for the Upgrading of Naphtha

(which heats the load with the stream coming out of the reactor). This action of heat integration is done to minimize the heater's energy requirements.

The preheated oil is sent to the feed heater, which heats it to a temperature of 450°C. This heated oil is ready to be reacted in the hydrotreater. The conditions are 8.8 MPa, 450°C, a Liquid Hourly Space Velocity (LHSV) of 1.11, 0.46 and 0.87 h⁻¹, and a hydrogen-to-oil ratio consumption calculated of 450, 500 and 600 ft³/bbl at STP for naphtha, gas oil and bottom cases, respectively.

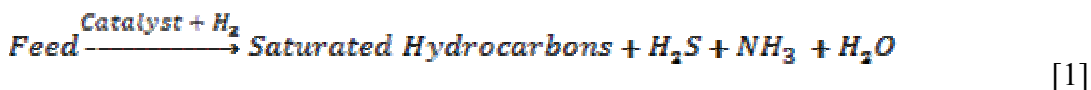
After the oil blend is upgraded, it is sent into the heat exchanger to cool it down. The high pressure flash separator operates at a temperature of 122°F and a pressure drop of 10 kPa; it splits the liquid oil and the gaseous hydrogen, sulfur and nitrogen content. Ninety-seven percent of the vapor stream (consisting mostly of hydrogen) is recycled back to the reactor, purified in a flash unit, heated and recompressed, whereas the liquid is mixed with the other blends, stored and sent by pipeline to a refinery.

2.3.4.1 Hydrotreating Reactor

A catalytic isothermal plug flow reactor is used to upgrade and treat raw oil blends into lighter and purer products. The LHSV for oil was determined from the kinetics involved in this process. Additionally, since the reaction is endothermic, heat is provided to the reactor by using either an oxy-fired or an air-fired furnace. Preheated recycled, made-up hydrogen and oil, are fed into the reactor where the processes of hydrodesulfurization (HDS), hydrodenitrogenation (HDN) and hydrogenation of aromatics (HDA) take place. The reactor effluent is sent into a flash unit, where H₂, H₂S, NH₃ and other gases are removed and recycled back into the reactor.

2.3.4.2 Catalytic Reactor Kinetics

Determining every single reaction that occurs during the hydrotreatment process is not reasonable. For that reason, a general chemical reaction is used to summarize the main aspects of the process. According to Owusu, this reaction can be written as (Owusu, 2005):



Although the general reaction implies the processes of HDN, HDS and HDA, it is still necessary to determine the kinetics for each process. Therefore, for the purpose of this simulation, while HDN and HDS were assumed to be first order kinetic constant models, HDA was assumed to behave as the lumped kinetic model shown in Figure 2.7.

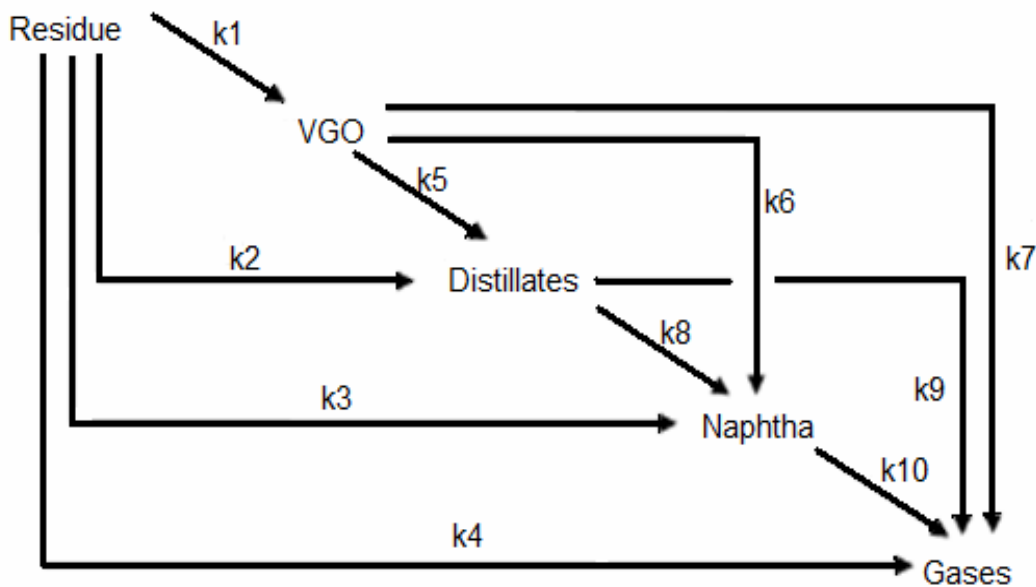


Figure 2.7: Kinetic Model for Hydrotreating, (Sanchez, 2005)

All of the kinetic constants and activation energies are shown in Appendix A-1 and are computed within the simulation for specific operating conditions. Since the kinetic model was used to determine the LHSV (which is required to determine the size of the reactor) that would achieve the desired conversion, conversion was defined as:

$$\% \text{ conversion} = \frac{EP_{feed} - EP_{product}}{EP_{feed}} = 1 - \exp\left[\frac{-k}{LHSV}\right] \quad [2]$$

where EP indicates the fraction of the substance in the feed or product boiling point above the desired endpoint. These boiling endpoints were classified as unconverted residues (1000.4 °F +), vacuum gas oil (VGO; 649.4-1000.4 °F), distillates (399.2-649.4 °F), naphtha (Initial Boiling Point (IBP)-399.2 °F) and gases.

The desired conversion was determined as the target characteristics of the oil that will be sent through the pipeline. After getting different LHSV values for each boiling endpoint, HDN and HDS, the smallest LHSV was chosen to be the operational condition for the reactor. The rationale for this is that the smallest LHSV implies the reaction limiting step or the reaction that takes the longest to occur.

To compute the volume of the reactor, it was necessary to consider the residence time of oil inside the reactor, the volume of hydrogen present at operational conditions and the catalyst volume.

The volume of the catalyst required in the reactor is a function of the oil volumetric flow and the LHSV chosen:

$$V_{\text{catalyst}} = \text{Volumetric Flow Rate of Oil/LHSV} \quad [3]$$

The hydrogen consumption was calculated using the graphical method that is shown in Figure 2.8 and was used as follows. Considering the composition of an oil blend to upgrade, with a sulfur removal of 0.69 wt%, a nitrogen removal of 1.8 wt% and an olefin crack of 38.61wt% and a flash operating at a pressure over 1200 psi; the total hydrogen consumption was estimated to be of 500 scft/bbl of oil.

Finally, an additional 10% was added to the reactor volume for an overdesign contingency.

2.3.4.3 Energy and Mass Balances

To keep the reactor isothermal, an energy balance was required, considering the enthalpy flow rate in and out of the reactor, as well as the heat consumed per pound of material reacted ~220 Btu/lb (Wilson, 1997) and the hydrogen heating requirement. A burner was simulated to produce the heat requirement for the reactor and the feed heater.

2.3.4.4 Burner Configurations

The air and oxy-fired burners used in this project have different configurations. The oxy-fired burner has a CO₂ recycle loop and recompression stage to compensate for any pressure drops. The purpose of this configuration is to lower the temperature of the burner to the adiabatic flame temperature of the regular air-fired burner. The process flow diagrams for both furnaces are depicted in Appendix A-2 and A-3.

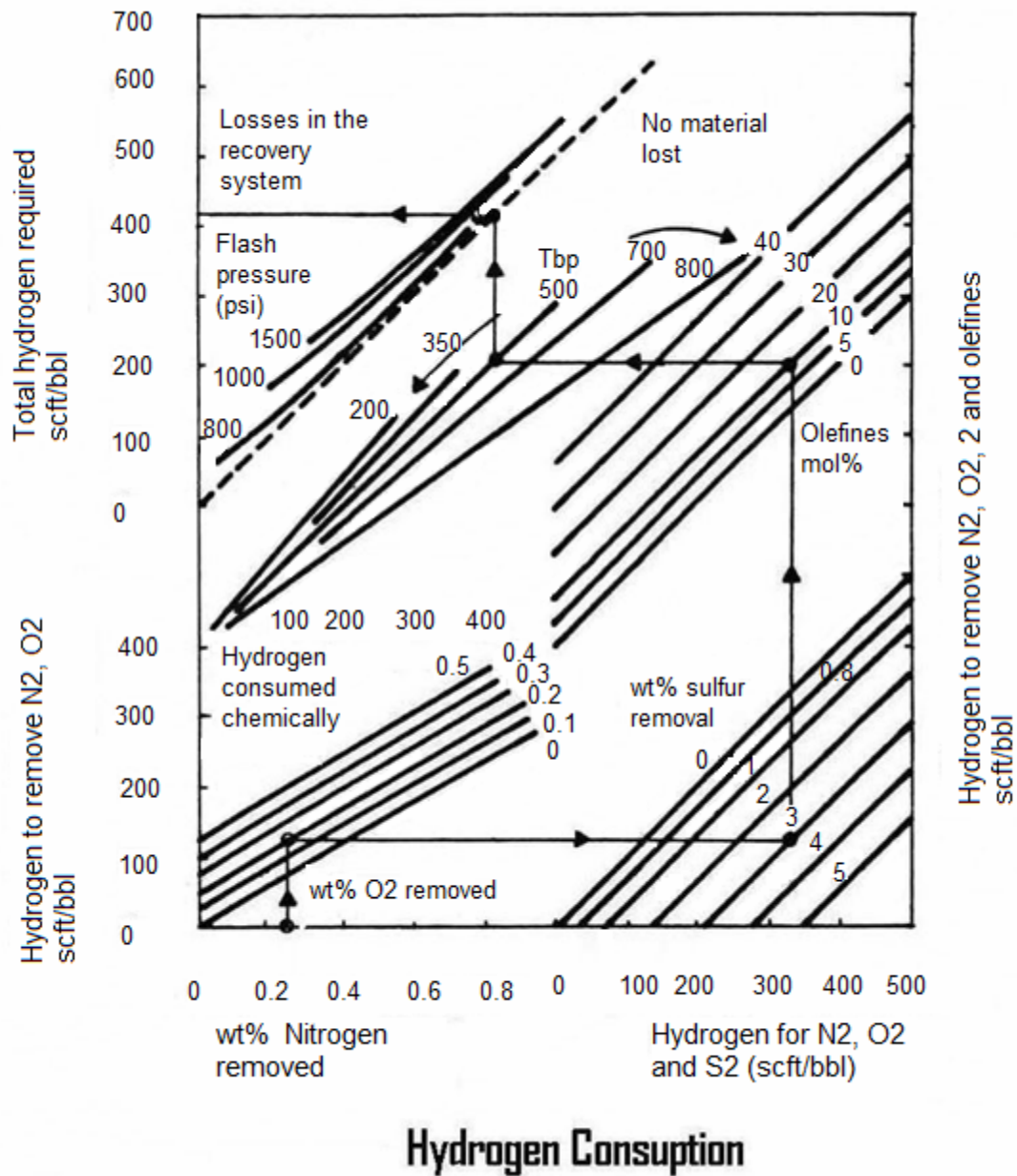


Figure 2.8: Hydrogen Consumption Chart, (Instituto Mexicano del Petroleo, 1979)

These reactors are specified to react stoichiometrically with an inlet temperature of 674°F and atmospheric pressure. The efficiency of the reactor is dictated by the flue gases temperature which was specified as 650°F, (Seider, 2004). The reason for this temperature is to avoid condensation of the flue gases and consequent corrosion.

2.3.5 Hydrogen Plant

In order to upgrade the shale oil to the point where it can be pumped in a traditional pipeline hydrogen has to be added to the crude. Assuming that the shale oil is produced from a commercial scale operation located in the Green River Basin, an estimated of 1.94 kg of H₂ /bbl must be added to the oil.

The hydrogen plant utilizes a natural gas boiler, methane steam reformer, water-gas shift reactor and two flash tanks for H₂ separation. See Figure 2.9 for a process schematic. The process uses natural gas, oxygen and water as feeds to produce H₂ in three steps. The key step for producing hydrogen is given in Eq [4]:



However, this reaction is endothermic and requires a large amount of heat. The primary source of that heat (and of an additional amount of H₂) comes from the partial combustion of natural gas in a gasifier:

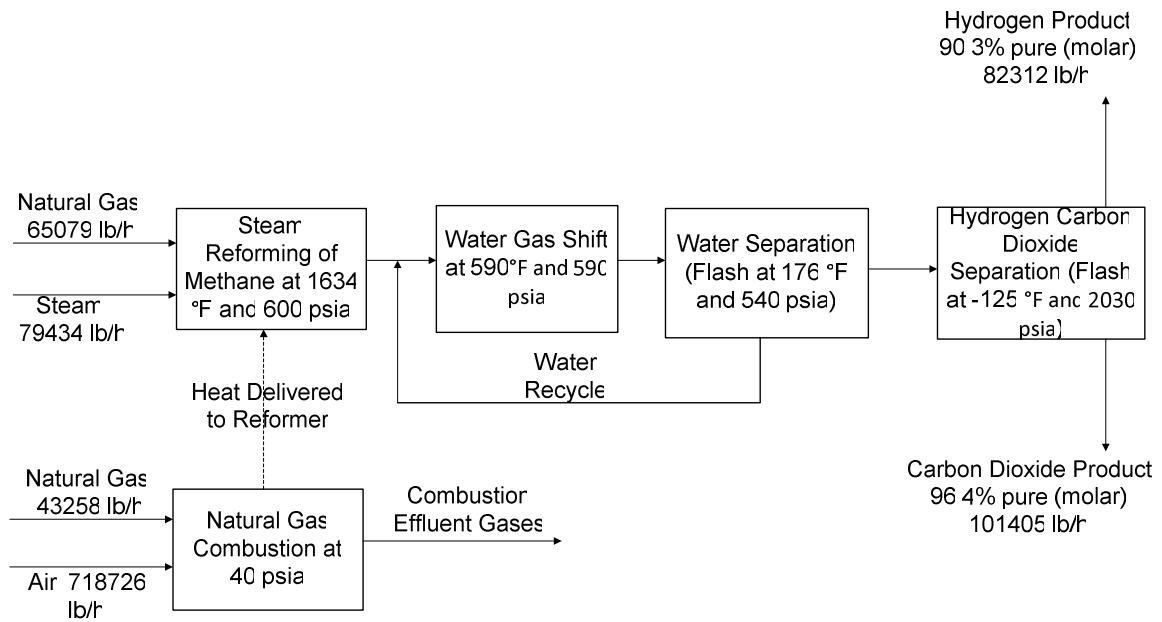
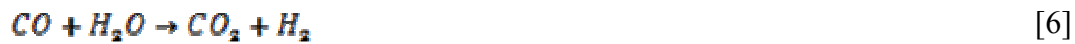


Figure 2.9: Block Diagram Describing the Overall Natural Gas to Hydrogen Process.



Finally, CO in the syn gas from both the steam reformer and gasifier can be combined with water in a water-gas shift reaction:



Water-gas shift reactions are typically carried out in two stages with a high (350°C) and a low (200°C) temperature step. However, in our design, we found that acceptable levels of CO conversion were achieved without the low temperature step.

Environmental concerns include the formation of hazardous pollutants such as NO_x , SO_x , particulate matter, H_2S and CO . However, perhaps the biggest environmental concern is the amount of water that this process could consume.

Water usage is negligible compared to the average flow of the Green River (the nearest major water source), which is approximately 3,950 Mgal/day (Enright, 2005); if oil shale development accelerates in the Green River Formation, water usage could become a serious issue.

Steam reforming of methane is used to convert natural gas to hydrogen and carbon monoxide. This process takes place at 1634 °F and 600 psia. Steam is fed in excess to the process to push the equilibrium in favor of hydrogen and carbon monoxide. Ninety-seven percent of the methane is converted in this process. The heat for this reaction is generated from combustion of natural gas in another reactor. The effluent from the steam reformer is combined with additional steam and fed to a water gas shift reactor, which takes advantage of the carbon monoxide in the stream by oxidizing it and reducing water to form more hydrogen. The water gas shift takes place at 590 °F and 590 psia and results in conversion of 94% of the carbon monoxide to form additional hydrogen.

The effluent from the reaction sequence is then cooled to 176 °F, where most of the water is removed by a flash tank. This water is 99.8 % pure and can be recycled back to the water gas shift process, which requires excess steam so that the equilibrium favors the hydrogen product. The carbon dioxide and hydrogen are then separated by a high pressure and low temperature flash, which results in a stream that is 90.3 % pure hydrogen. Although this process requires large amounts of refrigeration to reach the very low temperatures required to condense carbon dioxide, this was deemed to be the most

economical CO₂ removal technique because it does not require large solvent flow rates or the equipment necessary for an absorption/stripping process.

2.3.5.1 Steam Reformer

The Natural-Gas-to-Hydrogen Process uses steam reforming of methane to convert natural gas to carbon monoxide and hydrogen. This process is endothermic and requires large amounts of heat to reach the activation energy required for the reaction to proceed at significant rates. The reaction consumes 447,000 kJ for every kmol of methane that reacts, so the feed entering the reactor or the reactor itself must be heated to achieve significant yield for the process. The reactants enter the process at 1,634°F and the reactor is also heated to maintain that temperature, as the reaction itself consumes energy. The stream consumes heat and the products leave the reactor at a temperature of 1,634.4°F. This setup requires a reactor with a heating jacket and some type of heat transfer fluid, such as a molten salt, to deliver the heat to the reactor. The heat source for this reaction comes from combustion of natural gas, which takes place in a furnace (labeled NG Combustion in the process flow diagram). The molten salt would be heated in the furnace and then transferred to the Steam Reformer to provide the necessary heat. A schematic of this process is shown in Figure 2.10. The process was modeled so that the energy generated from the natural gas combustion process was equal to the energy required by the steam reforming process.

Because the reaction is reversible, large amounts of steam (54% of the feed molar) are used to push the equilibrium toward the products, carbon monoxide and hydrogen.

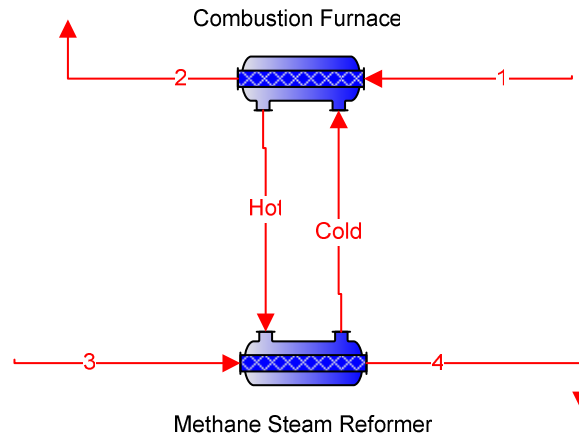


Figure 2.10: Using Heat Transfer Fluid to Heat the MSR Process from the Combustion of Methane

Although adding pressure does not favor the formation of products in the reaction, it does make the reaction happen at a higher rate by increasing the partial pressure or concentration of each component. Thus, the reactants are fed to the reactors at a pressure of 600 psia. The reaction uses a zinc-stabilized copper catalyst with a density of 4,000 kg/m³.

The Methane Steam Reformer (MSR) converts 97.7% of the methane to carbon monoxide and 76.9% of the water. The excess water is not problematic, however, as it can be used in a water-gas shift reaction to obtain more hydrogen from the remaining carbon monoxide, as will be discussed later. The mass flow rates of each component in the reactor as a function of distance down the reactor (shown in 10 increments) are shown in Figure 2.11.

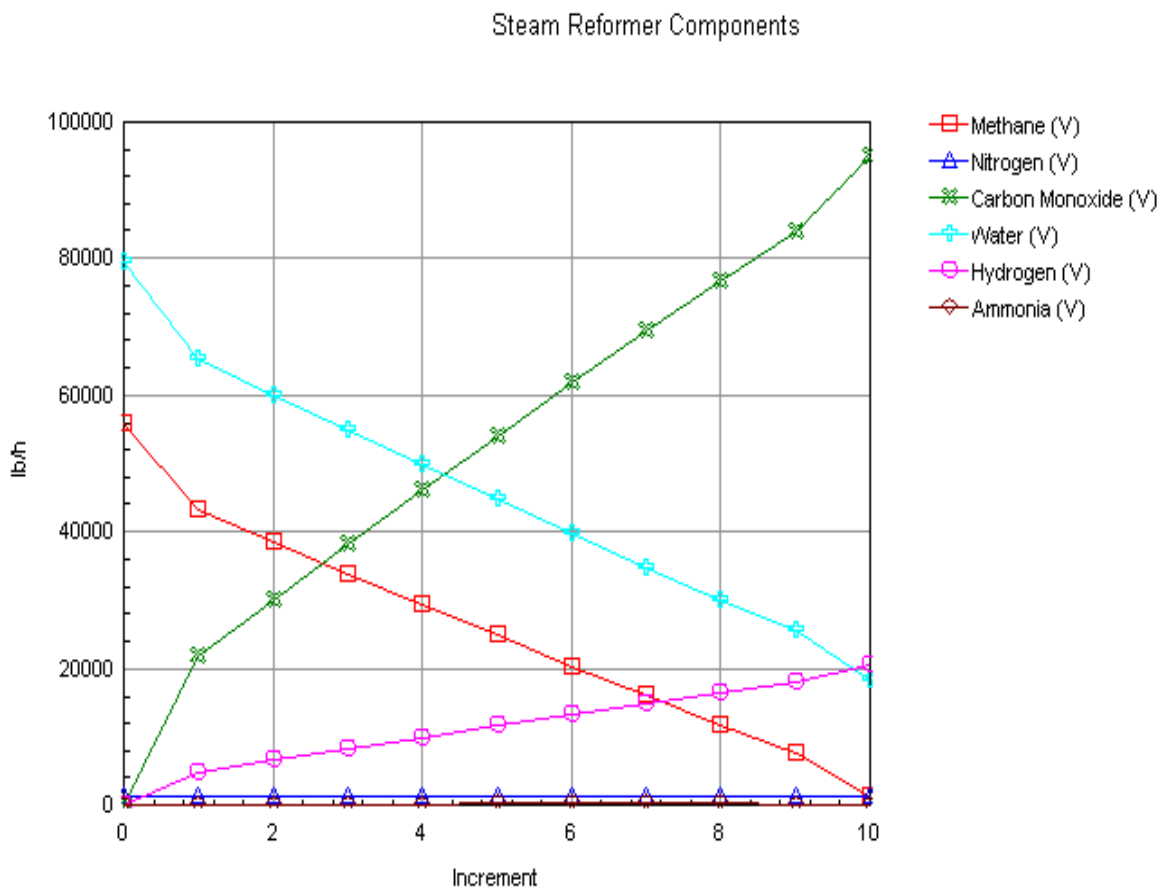


Figure 2.11: Flow Rates of each Component in the MSR Reactor as a Function of Distance Down the Reactor (Shown in 10 Increments)

Steam reforming has several advantages over the gasification of natural gas. The process, while energy intensive, produces three moles of hydrogen per mole of methane, as opposed to two for gasification processes. The process does not require oxygen, which must be of high purity and is very expensive. Instead, steam is reacted with methane to form the CO and H₂ products. Additionally, because there is no oxygen entering the reactor, the side reactions:

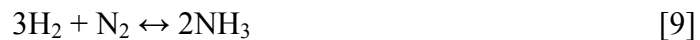


do not consume the desired products, and greater yield of H₂ and CO can be achieved.

The process does have disadvantages compared to gasification, however. The steam reforming process does nothing with the heavier hydrocarbons in the natural gas. Also, gasification is highly exothermic and does not require utilities to heat the streams. In fact, the energy from the gasification reaction can be used to heat other streams or generate steam for electricity generation.

2.3.5.2 Ammonia Formation

Another reaction added to the reaction set for the steam reformer was the formation of ammonia from hydrogen and nitrogen.



In order to quantify the formation of ammonia, this reaction was added to the reaction set for the steam reformer. It was assumed that the reaction is governed by equilibrium.

2.3.5.3 Water-Gas Shift Reactor

The water-gas shift reaction can be used to form additional hydrogen from carbon monoxide by the reaction:



Reactants enter the reactor at 590°F and exit at 781.6°F since the reaction is exothermic. The inlet pressure is 590 psia and the reactor has a 10 psia pressure drop. Additional water is added to the feed stream to push the reaction further toward the formation of carbon dioxide and hydrogen. The reactor uses an iron oxide catalyst that is promoted with chromium oxide with a density of 1300 kg/m³. The mass balance for this reactor is shown in Figure 2.12.

The reactor has a conversion of 94% based on carbon monoxide, which is the limiting reactant. Because of this high rate of conversion, another water-gas shift reactor is not used. It proves to be very difficult to get additional conversion from the carbon monoxide as the large amounts of hydrogen and carbon dioxide already in the stream push the equilibrium in favor of the reactants. A more detailed process flow sheet with a table for properties and composition of each stream is given in Appendix A-6.

2.3.5.4 Gasification vs. Steam Reforming

Natural gas can be converted to hydrogen and carbon monoxide by two different reactions: methane steam reforming or gasification. Each reaction forms hydrogen and carbon monoxide with the reactions shown below:



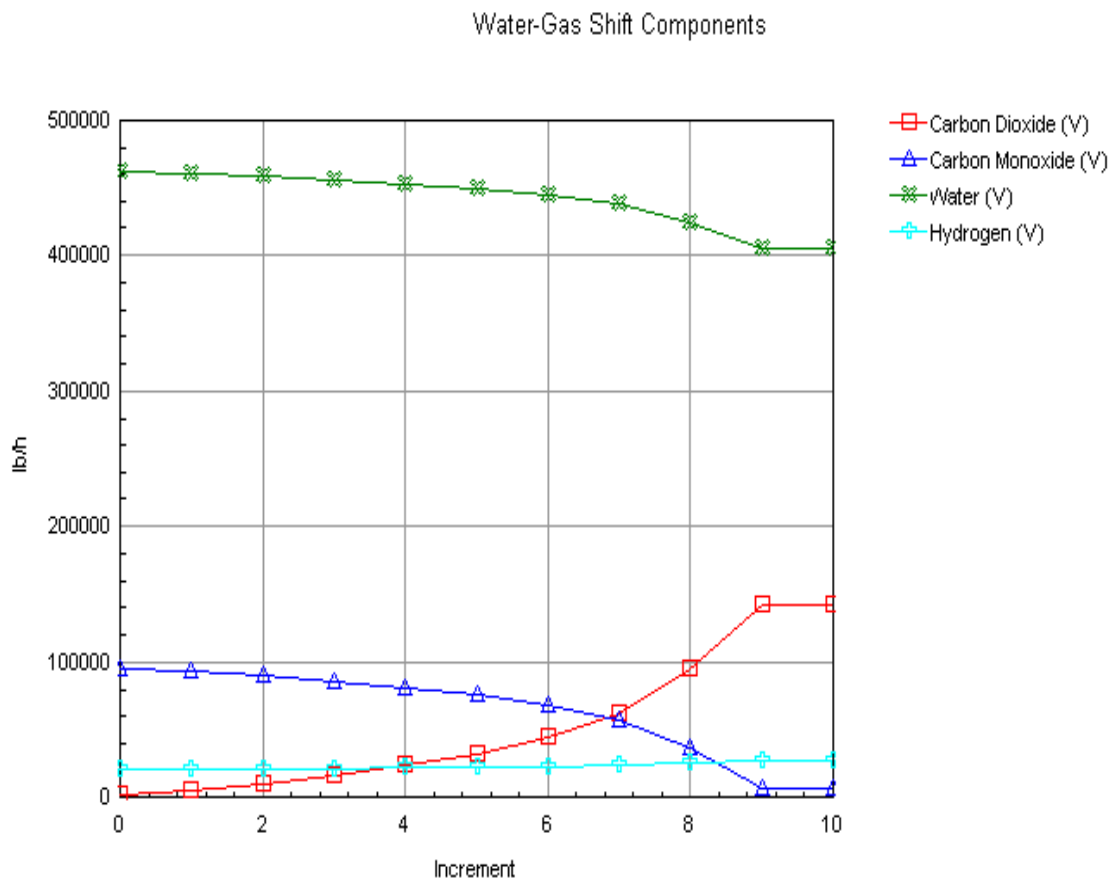


Figure 2.12: Mass Flow Rates of each Component in the Water-Gas Shift Reactor as a Function of Distance Down the Reactor (Shown in 10 Increments)

Steam Reforming: $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$

[12]

Because either process seemed to be a viable candidate for hydrogen production, a study was undertaken to select a reaction before any system design was begun.

Each process has advantages and disadvantages. Steam reforming of methane uses water rather than oxygen as a reactant. Because buying pure oxygen is rather expensive, using water instead can be beneficial. The steam reforming process also

generates three moles of hydrogen per mole of methane as opposed to two for the gasification process. A disadvantage of steam reforming is that it is endothermic and requires large amounts of energy to power the reaction to completion.

The gasification process, however, is exothermic and the energy liberated by this reaction can be used to save energy elsewhere in the process. Gasification also takes advantage of the larger hydrocarbons (ethane, propane, butane, etc.) to create more carbon monoxide and hydrogen, while steam reforming does not take advantage of these compounds.

A disadvantage of gasification is that pure oxygen will also react with carbon monoxide and hydrogen to form undesired products, carbon dioxide and water, respectively. These side reactions must be minimized or they will result in significant yield loss of the hydrogen product. In order to estimate which process would be more cost-effective, an economic analysis was undertaken to determine the cost per hydrogen produced. This analysis assumed that natural gas was pure methane (92.6% in reality) and that no side reactions occurred. The energy generated or consumed was considered an energy savings or cost, based on the cost and heating value of the methane. Thus, it was assumed that the energy required by the steam reforming process would come from combustion of natural gas. Based on the costs given for each material, it was determined that steam reforming, despite its endothermic nature, was more cost-effective, as shown in Table 2.5.

The reactions could also be run in parallel with the heat from the gasification process being delivered to the steam reforming process.

Table 2.5: An Economic Summary of Gasification vs Steam Reforming for the Natural Gas to Hydrogen Process.

	CH ₄ /H ₂	O ₂ /H ₂	H ₂ O/H ₂	kJ/H ₂	\$/kmolH ₂
Gasification	1/2	1/4	0	-17840	\$3.28
Reforming	1/3	0	1/3	149324	\$2.84

Based on the heat of reaction of each process, gasification would have to be done in approximately a 9:1 ratio to reforming to balance the heat duty of each process. The economic summary for this combination is given by Table 2.6.

Based on these preliminary estimates, the steam reforming reaction was chosen. This reaction would be powered by the combustion of natural gas using a heat transfer fluid, such as a molten salt, to transfer heat from one reactor to the other.

2.3.5.5 Environmental Assessment of Hydrogen Plant

A number of methods have been proposed by Allen and Shonnard (Allen, 2002) for quantifying the environmental impact of chemical processes.

Table 2.6: An Economic Summary for Using Gasification and Steam Reforming in Parallel, Using the Energy Generated from Gasification to Heat the Steam Reformer.

	% of Total	CH ₄ /H ₂	O ₂ /H ₂	H ₂ O/H ₂	\$/kmolH ₂
Gasification	89.33%	1/2	1/4	0	\$3.28
Reforming	10.67%	1/3	0	1/3	\$2.84
				Total Cost	\$3.23

Typically, the first step in comparing the environmental impact of a process is to compute the processes environmental index (EI) based on toxicity:

$$EI = \sum v_i \left(\frac{1}{TF_i} \right) \quad [13]$$

where v_i is the stoichiometric coefficient of species i and TF_i is a toxicity factor (usually the threshold limit value, TLV, or permissible exposure limit, PEL) for the compound. Unfortunately, implementation of this initial approach is complicated by all of the different reactions considered in each process flow sheet, and is not particularly useful because each process involves almost exactly the same chemical species. Even without performing any calculations, it is clear that according to Eq [13], the steam reforming process will be more environmentally friendly than gasification of shale oil because of the heavier hydrocarbons and sulfur content of the shale oil feed.

A more applicable method developed by Allen and Shonnard (Allen, 2002) is to compare the mass and emissions required to produce a unit of product. Using 1lb of H_2 product as the basis for comparison, steam reforming and gasification of shale oil are compared in Table 2.7 (the data used in the analysis below was taken from each process flow sheet)

As illustrated in Table 2.7, steam reforming is again the preferred process in all categories. The results in Table 2.7 can be intuitively understood by considering the

Table 2.7: Environmental Comparison of Steam Reforming and Shale Oil Gasification. Emissions Include all Gaseous Products except CO₂.

Process	Intensities (lb/lb H ₂)			
	Material	Water	CO ₂	Emissions
<i>Steam Reforming</i>	9.71	1.02	9.49	0.22
<i>Shale Oil Gasification</i>	14.66	2.41	13.76	0.96

hydrocarbon feedstock used for each process. More material is required to produce the same amount of H₂ with shale oil gasification because the mass fraction of hydrogen to carbon atoms is lower in shale oil than in natural gas. It should also be noted that shale oil gasification requires almost 1.5x as much water as steam reforming. As mentioned previously, water usage is a major issue in the Green River Basin area, and such a significant reduction in the use of water points to yet another advantage of steam reforming over shale oil gasification.

2.3.5 Pipeline and Pumping Stations

After the hydrotreating process, the upgraded oil blends are mixed and decompressed and sent through a pipeline. The pipeline for this process runs from the mining site (close to Bonanza) to Vernal and then to North Salt Lake, UT. The mine location has coordinates of 39°57'02.33"N and 109°10'03.68W, and has a distance to Vernal of 37.27 miles and there is negligible elevation change. The total length was estimated to be 379.57 km. The inlet and outlet pipeline pressures were assumed to be atmospheric and temperatures were taken to be 20°C. The pipe was buried at 3 ft below the ground surface. From the features of the oil and the environment, it was estimated

that an economical pipeline diameter could be 12 in. The material of the pipe was assumed to be Carbon Steel A134.

The optimal pipe diameter was computed by optimizing the pumping requirements and costs. For a given flow rate, larger pipe diameters reduce pumping costs by lowering the velocity of the flow resulting in lower Reynolds numbers and consequently low friction factors. Conversely, larger diameters increase capital costs, which are proportional to the amount of steel in the pipe. Therefore, from the approach suggested by Nolte (Nolte, 1978), the economical diameter was taken as:

$$D = \frac{W^{0.44s} \mu^{0.02s}}{\rho^{0.31s}} \left[\frac{0.0657 Y K}{(a + b)(F + 1) X E} \right]^{0.15s} \quad [14]$$

where:

D= economically optimum pipe internal diameter, inches

W= Flow rate, thousands of pounds per hour

μ = Viscosity of the fluid, centiPoises

ρ = Density of the fluid, pounds per cubic foot

Y=Hours of operation per year

K= Cost of power, \$0.04/kWh

a= Amortization rate, reciprocal of years ~0.03

b= Maintenance fraction, 0.5

F= Factor for cost of fittings, valves and erection compared to bare pipe cost

X= Cost of 1 ft of 2 in schedule 40 carbon steel pipe, \$1.08 / ft

E= Pump efficiency, 80%

For higher accuracy in the simulation, it is necessary to consider any elevation change in the selected route (see Figure 2.13). From Vernal to mile 71, an average inclination angle of 0.013° was calculated, while the remaining distance was specified with an inclination angle of -0.0196 .

The pumping requirements were automatically calculated to overcome any inclination, friction and oil hold ups by the use of standardized centrifugal pumps. Based on the maximum designable pumps (Seider, 2004) a total of four pumping stations were required.

The costs for the pipe and the pumping stations were computed based on Boyle's methodology (Boyle, 2002), which consisted of different steps. The first step required for this method is to get a base pipe cost in dollars (July 1992) per diameter-inch per lineal foot (\$/in/ft), using the following equation:

$$Cost = 2 + (Pipe\ Diameter - 36) \times 0.027 \quad [15]$$

Afterwards, some adjustments to this cost have to be made such as the consideration of pressure class, pipe installation and delivery (add~ \$3.30in/ft), depth of cover soil rippability, slope change, congestion and appurtenance factors, ENR cost index, climate and contingencies which used a suggested default of 25%.

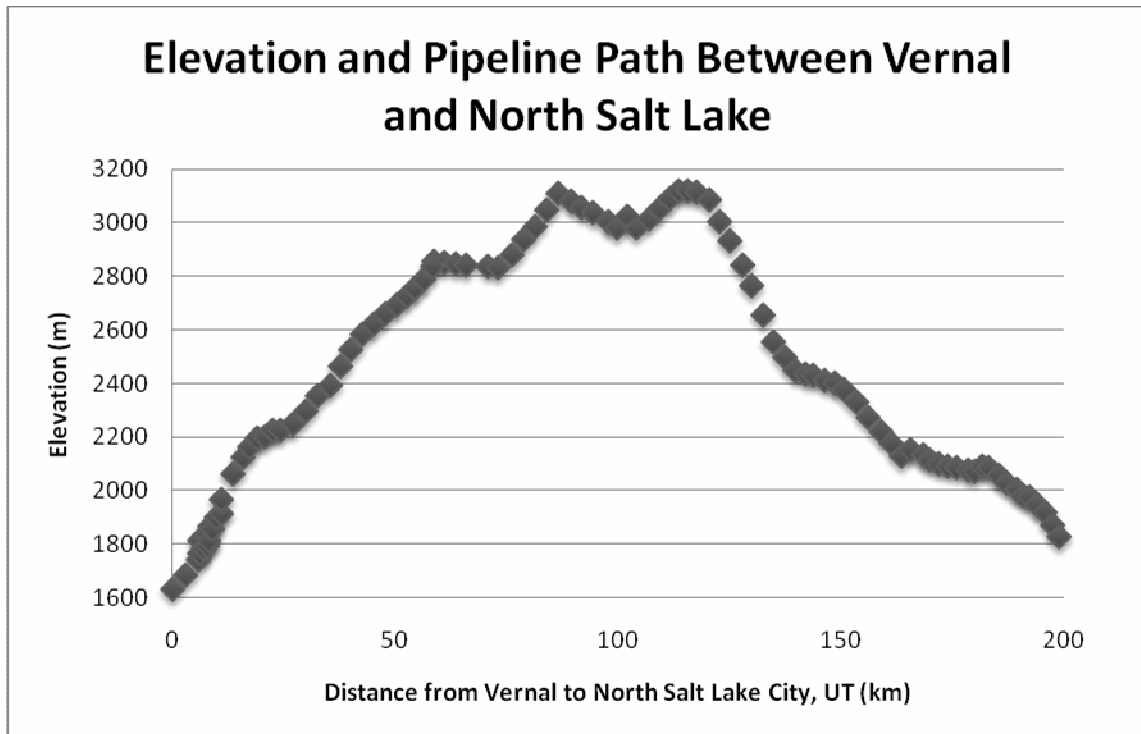


Figure 2.13: Elevation Change for Pipeline Design

The pumping station costs were estimated using, the following equation (Boyle, 2002):

$$C = 46000 \cdot \frac{Q^{0.75}}{100} \left(\frac{H}{300} \right)^{0.66} \quad [16]$$

where:

C is the total cost, (2001 US dollars)

Q= the flow rate, gallons per minute

H= the head, feet

2.3.6 CO₂ Compression System

The flue gases from the oxy-fired model are sent to a compression system before they are sent to the CO₂ pipeline for to sequestration. This compression system is divided into two stages: the purification stage of CO₂ and its compression/cooling section.

For the first section, the flue gases that are emitted by the hydrotreater's oxy-fired burner, the retort process and the hydrogen plant are mixed and sent through a series of heat exchangers with the purpose of condensing any water present and to isolate the CO₂ gas. While the two initial heat exchangers operate with cooling water, the third exchanger uses a refrigerant (R-134). The refrigerant is required to reach -10°F and produce a CO₂ purity of 99.9 wt%. After the cooling process, the emissions are sent to a flash vessel, where water is condensed and the separation is produced.

The purified CO₂ is then sent to a system of compressors and heat exchangers with the purpose of reaching the CO₂ critical point (35°C and 7.6 MPa), where its volume has been significantly reduced and ready to be sent through a pipeline. The utility used in the heat exchangers for cooling in this process was water which entered at a temperature of 32°C and a pressure of 20 psia and left at 49°C. All of the hot water produced in these two systems is collected and recycled. The refrigerant enters at -102°C and 25 psia and leaves at -98°C. For a process diagram describing this process, see Figure 2.14.

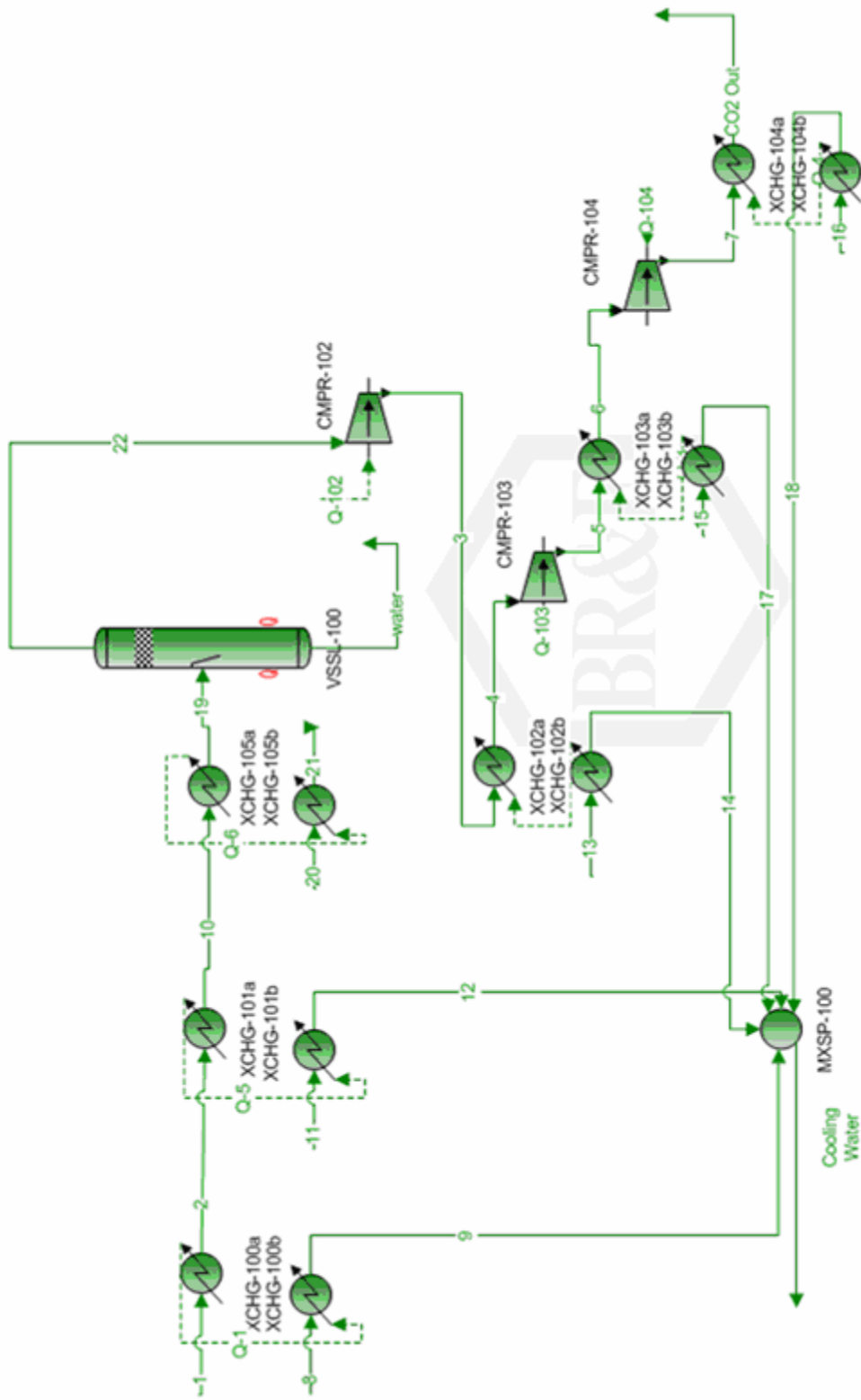


Figure 2.14: Process Flow Diagram for CO₂ Compression System

2.3.7 Water Reservoir

The extraction and upgrading process requires water on a daily basis as well as a one time supply to fill tanks to start up operations. Due to the requirement for the process, plants need to operate “24-7” over an annual operating schedule of 330 days/y, water for the various processes, especially for steam generation, must be available. Water is estimated to cost \$50/ac-ft/yr in this region. It must be purchased from other users since they are available in the region. Since water is a scarce commodity in this arid region of the west, a reservoir is needed.

The reservoir will be filled by either pumping water from the aquifer or by diversion of the Green River in the area to fill the reservoir. The size this reservoir needs to be is determined by the duration of a prolonged drought in the area. While this study has not done a sophisticated analysis of the hydrology of the Green River basin, we have taken a look at historical periods of drought as defined between the rain storms over the basin and found that 90 days or the duration of the summer is reasonable as a worst case for water storage.

As a result of the total water utilization for the process being 3500 ac-ft/y for the air-fired combustion heating case and the need for a 90-day supply, the size of the reservoir is determined. From the size of the reservoir, the cost can be determined using construction excavation costs that are applicable in this part of the state of Utah (RSMMeans, 2002). The cost of a water reservoir for this operation is substantial, as we will see.

2.3.8 Utility Plants

Each of the utilities used throughout the processes requires a source; for that reason, utility plants, pipelines, electric lines and others were sited and their costs were estimated.

The costs for the substations were computed based on Seider's methodology (Seider, 2004), where the investment costs were related to the rate of usage for each facility (Table 2.8.)

Additionally, the costs for the electric and gas lines were assumed to be \$425,000/mile and \$200.00/ft, respectively, the electric switching, gear and tab, \$10,000/mile, and the meter and regulation facility for natural gas, \$1,000,000. The location to the closest service facility was assumed to be in Bonanza UT (about 5 miles).

Table 2.8: Allocated Capital Investment Costs (Seider, 2004)

Utility	Capital Cost Rate
Steam	\$50/(lb/hr)
Electricity	\$203/Kw
Cooling Water	\$58/gpm
Process Water	\$347/gpm
Refrigeration	\$1,330/ton
Liquid waste disposal	\$3/1,000gpy

CHAPTER 3

EQUIPMENT SIZE AND COSTING PROCEDURES

3.1 Introduction

In order to determine the economic viability of the processes and scenarios described above, it was necessary to calculate annual cash flows. These cash flows were estimated for each year for a period of 20 years. These cash flows were calculated as follows:

$$CF = P \cdot S - P \cdot C_v - C_f - T - C_{TDC} \pm C_{WC} - C_L - C_S - C_R + S_{equip} \quad [17]$$

$$T = t(P \cdot S - P \cdot C_v - C_f - P \cdot d - D) \quad [18]$$

where:

CF= Annual cash flow

C_v = Variable operating costs

C_{TDC} =Total depreciable capital

C_S =Cost of start up

P= Production capacity (days operated/yr)

C_f = Fixed operating costs

C_{WC} =Working capital

CR= Cost of royalties

S=Total gross sales

T=Taxes

C_L =Cost of land

S_{equip} = Equipment salvage

T=Corporate tax rate

d=Depletion

D=Depreciation

Each term represents the amount of revenue or costs in that category in a given year. The present value (PV) of the cash flow in each year of project was determined by applying the discount factor:

$$PV = CF \left[\frac{1}{(1 + i)^n} \right] \quad [19]$$

which adjusts the cash flow in the n-th year of a project according to an annually compounded interest rate i (representing the time-value of money for the entity financing the project). The net present value (NPV is the summation of each year's present value cash flow) and the internal rate of return (IRR is the interest rate i that results in NPV = 0) for each scenario were computed to assess profitability. Individual terms in Eq. [15] – [19] was evaluated as discussed below.

3.2 Capital Costs

Capital costs for the project were estimated using a combination of two techniques: namely, William's six-tenths rule (Williams, 1947) for economy of scale and the individual factors method of Guthrie (Guthrie, 1974).

According to Williams (Williams, 1947), economies of scale in chemical processes (for everything from individual pieces of equipment to entire plants) can be described by Eq. [20]:

$$C = C_o \left(\frac{Q}{Q_o} \right)^m \left(\frac{I}{I_o} \right) \quad [20]$$

where C is cost, Q refers to a material capacity (oil production rate, raw shale processed, etc.), m is a scaling power, I is an appropriate cost index (CE Plant Index, Producers Price Index, etc.) and the subscript "o" refers to the base value of the subscripted variable. Equation [20] is referred to as the "six-tenths rule" because Williams (1947) found that on average, the best fit to cost data was given by $m = 0.6$, and for the purposes of this study, it was assumed that $m = 0.6$ for all capital costs (Eq. [20] was also used in some instances for estimating annual costs in which case $m = 1$, see the discussion of annual costs below). William's (1947) six-tenths rule was applied in the *ex situ* oil shale scenario to scale the capital costs and processing data for mining and retorting from Weiss (1982), whose work estimated the costs for producing 46,400 bbl/day of crude oil from oil shale using the TOSCO II process.

The individual factor method of Guthrie (1974) gives preliminary estimates of the C_{TDC} of a project based on the sum of the purchase costs (C_P) of individual pieces of

equipment multiplied by a series of factors to give a bare-module cost (C_{BM} , which accounts for the total direct (C_P) and indirect (delivery, insurance, taxes, installation, etc.) costs of process equipment):

$$C_{TDC} = \sum C_{BM} = \sum \left[C_P \left(\frac{I}{I_0} \right) [F_{BM} + (F_d F_p F_m - 1)] \right] \quad [21]$$

where each factor is:

F_{BM} = Bare-module factor

F_d = Design factor

F_p = pressure factor

F_M = material factor

Optimized process designs (including mass and energy balances, equipment sizing, and construction materials selection) were generated for the upgrading (hydrotreater and H_2 generation plant) and delivery (pipeline) portions of each scenario using ProMax (a process flow sheet simulator), which allowed for estimation of C_P from cost data given by (Seider, 2004) using the sizing factors specified in Table 3.1.

Taken together, the combination of William's six-tenths rule and the method of Guthrie provided reasonable estimates of the total depreciable capital cost (C_{TDC}) for each scenario. Other capital costs, such as the cost of working capital, land, startup and salvage were estimated as percentages of C_{TDC} as recommended by Seider (Seider 2004).

Table 3.1: Size Factor for Equipment Cost

UNIT	SIZE FACTOR	COMMENTS
Trickle-bed reactor	LHSV	NiMo/Al ₂ O ₃ Catalyst, kinetics from Botchwey (2004)
Pumps	Change in Pressure	
Heat Exchangers	Area	
Flash Separator	Residence Time	
Compressors	Horse Power	
Furnace	Heat Duty	
Steam Reformer	Residence Time	Cu/Zn Catalyst
Water Shift Reactor	Residence Time	Fe/Cr ₂ O ₃ Catalyst
Holding Tank	Volume	

Additional data and algorithms for estimating capital costs were used for offsite facilities not typically associated with the chemical industry. RSMMeans heavy construction cost data was used to estimate the cost of building a reservoir for process water (RSMMeans, 2002), and the approach suggested by Seider (Seider, 2004) was followed for approximating the cost of delivery pipelines.

3.3 Annual Costs

The annual costs in each scenario can be differentiated into fixed (C_F) and variable (C_V) costs based on whether they are or are not a function of the process being in operation.

Variable costs in our scenarios are defined as a combination of utilities (water, fuel, electricity, etc.) and other expenses related indirectly to production (sales, research, administration, etc.). Utility requirements were either taken directly from the appropriate process design flow sheet or scaled from base scenario process data (Weiss, 1982) for *ex situ* oil shale mine and retort) using a variant of Eq. [20]

$$U = U_o \left(\frac{Q}{Q_o} \right)^m \quad [22]$$

where U is the utility requirement and all other variables are the same as in Eq. [20], except that the scaling exponent m is always set to $m = 1$. Most utility costs were estimated from price data given by Seider (Seider, 2004), with supplementary price data coming from the EIA (2010), the Uintah Water Conservancy District (2010) and others. Estimates for indirect annual expenses were also derived according to Seider's recommendations.

The fixed expenses in the scenarios were assumed to be the cost of labor, property taxes and insurance, all of which were estimated according to Seider, who also suggested that property taxes and insurance were assumed to be a percentage of C_{TDC} (Seider, 2004). Labor was assumed to be a fixed expense because the large amount of manpower required during plant maintenance and downtime implies that operational labor would be participating in work during shut downs. Labor related to operations was estimated according to assumed hourly wages and the number of operators required for a sequence of process units based on the type of process (solids/fluids) that they handled and their throughput. Maintenance related labor was estimated as a percentage of C_{TDC} , again based upon the type of process handled.

3.3.1 Utilities to Operate *Ex Situ* Oil Shale

Utilities for this process are numerous. A list of utilities and their prices used for the *ex situ* extraction and upgrading of oil shale is given in Table 3.2.

Table 3.2: Utility Prices used for *Ex Situ* Extraction and Upgrading for Oil Shale

Utilities		
<i>Fuel (natural gas)</i>	\$ 4.27	per MBtu
<i>Electricity</i>	\$ 0.04	per kWh
<i>Water</i>		
<i>Raw water</i>	\$ 50.00	/ (acre-ft * yr)
	\$ 16,292.55	/ (k gal * yr)
<i>Water Storage</i>	90	days
<i>Water recycle loses</i>	3%	
<i>Boiler feed water</i>	\$ 1.50	/ k gal
<i>Process water</i>	\$ 0.50	/ k gal
<i>Cooling water</i>	\$ 0.05	/ k gal
<i>Steam</i>	\$ 5.50	/ k lbs
<i>Oxygen</i>	\$ 70.00	/ ton
<i>Catalyst</i>	\$ 4.24	/kg
<i>CO₂</i>		
<i>Tax Rate</i>	\$ 25.00	/ ton CO ₂
<i>Sale Rate</i>	\$ 25.00	/ ton CO ₂
<i>Refrigerants</i>		
<i>Ethylene: -150 deg(F)</i>	\$ 10.50	/ GJ
<i>R-134a: -30 deg(F)</i>	\$ 6.60	/ GJ
<i>Chemicals</i>	\$ 75.00	/ kg
Plant Utilization	330	days / year

3.4 Sales

Oil sales are calculated for each year of the project based on EIA (2010) forecasts. The sales price we have assumed for oil represents the refiner's acquisition price of imported low sulfur light crude given in the EIA's forecast. In addition to the sales revenue generated by oil, several scenarios also considered the possibility of implementing CO₂ capture. In these scenarios, free on board (f.o.b.) supercritical CO₂ sale for enhanced oil recovery (EOR) is included in each year's sales revenue at an assumed price of \$25/ton.

3.5 Taxes and Royalties

The total corporate state and federal taxes paid each year are calculated using Eq. [18]. Net income is calculated by subtracting all operating costs, depreciation and depletion from gross sales revenue. Depreciation of C_{TDC} is assumed to follow a 10-year Modified Accelerated Cost Recovery System (MARCS) schedule. If a given scenario involves a private land purchase for extracting oil and gas, then an additional deduction can be made for depletion (assumed to be 15% of gross income).

Royalties were assumed to start at 5% and increase up to 12.5% over a period of 10 years (Keiter, 2009).

CHAPTER 4

OPERATING COST AND ECONOMIC ANALYSIS

4.1 Air-fired Case

4.1.1 Capital Costs

The base case scenario for the oil shale production (quality of the rock of 25 gal/ton) revealed a total depreciable capital for this plant of \$3.34 billion. The largest capital costs are mining and retorting (71%), hydrotreater (23%), oil pipeline (4.8%) and utility plants (0.65%), in that order, along with only 1.08% which consists of the hydrogen plant, utility plants and the water reservoir. Figure 4.1 contains a pie chart of where the capital expenditures are depicted, while Table 4.1 contains the costs for each section of the process.

Additionally, the cases where the shale quality was 20 gal/ton and 35 gal/ton revealed capital costs of \$3.64 and \$2.97 billion, respectively. These results are reasonable; it was expected that the higher the quality of the rock, the less mining would be performed, and thus, the cheaper the overall process.

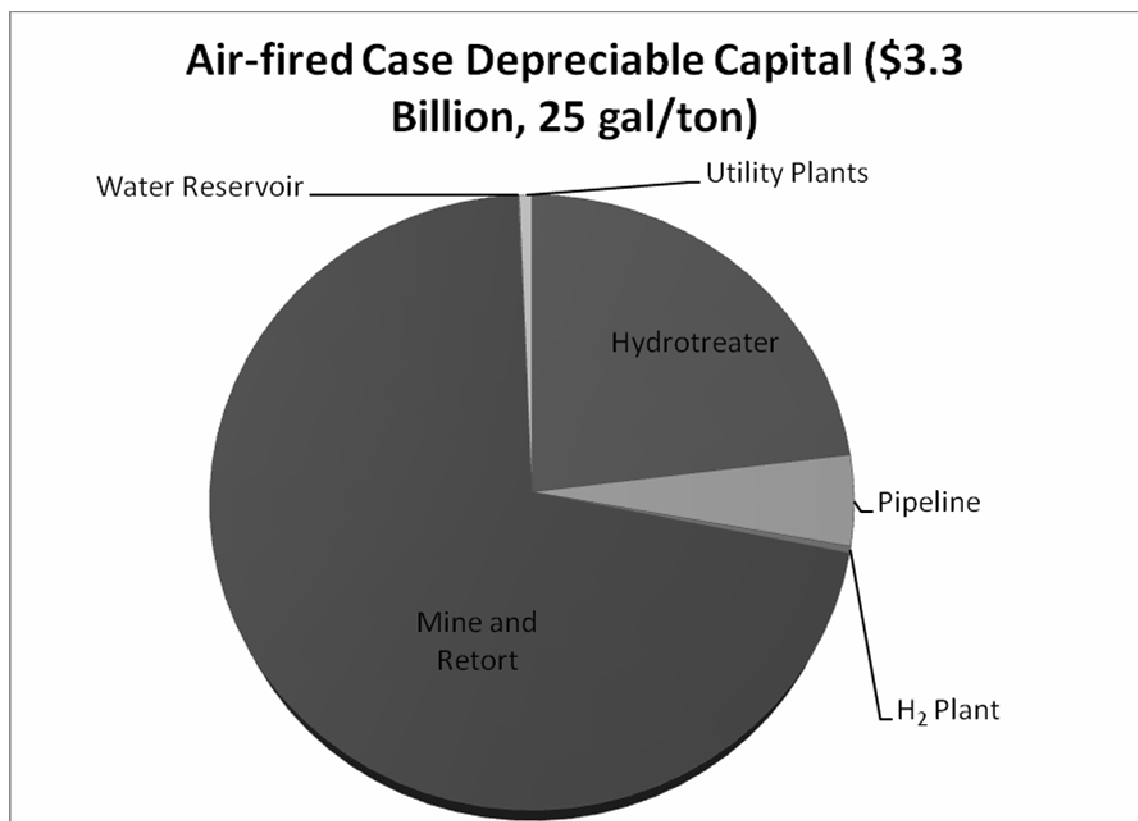


Figure 4.1: Pie Chart of Capital Costs for *Ex Situ* Oil Shale Extraction and Upgrading for Air-Fired Plant Heat Requirements

Table 4.1: Air-Fired Process Total Depreciable Capital for 25 gal/ton case

Hydrotreater	\$ 722,827,249.63	23.21%
Pipeline	\$ 148,923,634.96	4.78%
H ₂ Plant	\$ 11,200,985.49	0.36%
Mine and Retort	\$ 2,229,060,359.91	71.58%
Water Reservoir	\$ 2,172,261.83	0.07%
Utility Plants	\$ 20,224,670.92	0.65%
Subtotal	\$ 3,114,184,491.82	100.00%
Total	\$ 3,345,615,982.09	

4.1.2 Annual Sales and Costs

The total annual operating costs for the 25 gal/ton case was estimated at \$984 million with \$439 million in fixed costs and \$545 million in variable costs. Among these annual costs, the highest costs are labor (38%), general expenses (24%) and fuel (19%). Note that general expenses consist of sales expenses, direct research, allocated research, administrative expenses and incentives

Revenues for the base case and its variants are presented in Figure 4.2. Here we see two bars, one for revenue (R) and the other for costs (C) for this base case. As can be seen comparing the “R” and “C” bars, the revenue and the costs are equal, as they should be. The variable and fixed costs to produce the syn crude oil are broken down in the C bar. Starting from the top C-Base bar we find that the largest costs are for Profit (ROI) due investors corresponding to \$30.31/bbl to earnings, \$29.88/bbl of variable annual costs, federal taxes (assuming that the full rates are paid) corresponding to \$16.13/bbl and \$12.51/bbl for royalties, plant startup and land. The annual fixed costs correspond to \$12.36/bbl, while the interest charges on the total depreciable capital is \$11.11/bbl.

There are other subcategories within the variable cost, being general expenses such as direct and allocated research, management incentive compensations and administrative expense at 43.41 % and fuel (natural gas) at 34.3% the biggest. For the base case, these costs are broken down into percentages of the total variable cost in the pie chart shown in Figure 4.3 and Table 4.2.

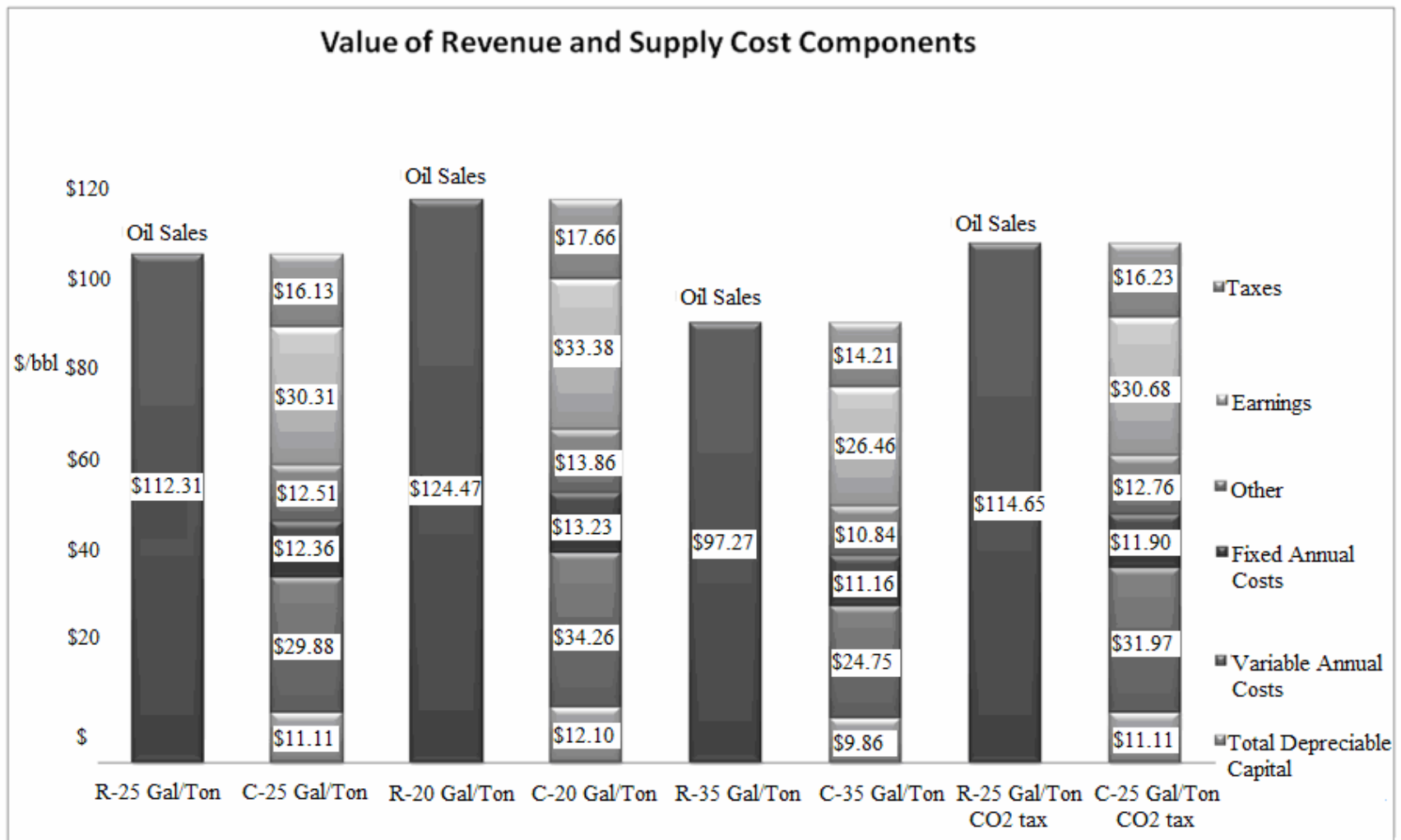


Figure 4.2: Revenue and Cost of *Ex Situ* Oil Shale Extraction and Upgrading for Air-Fired Plant Heat Requirements-Variable Grade of Oil Shale

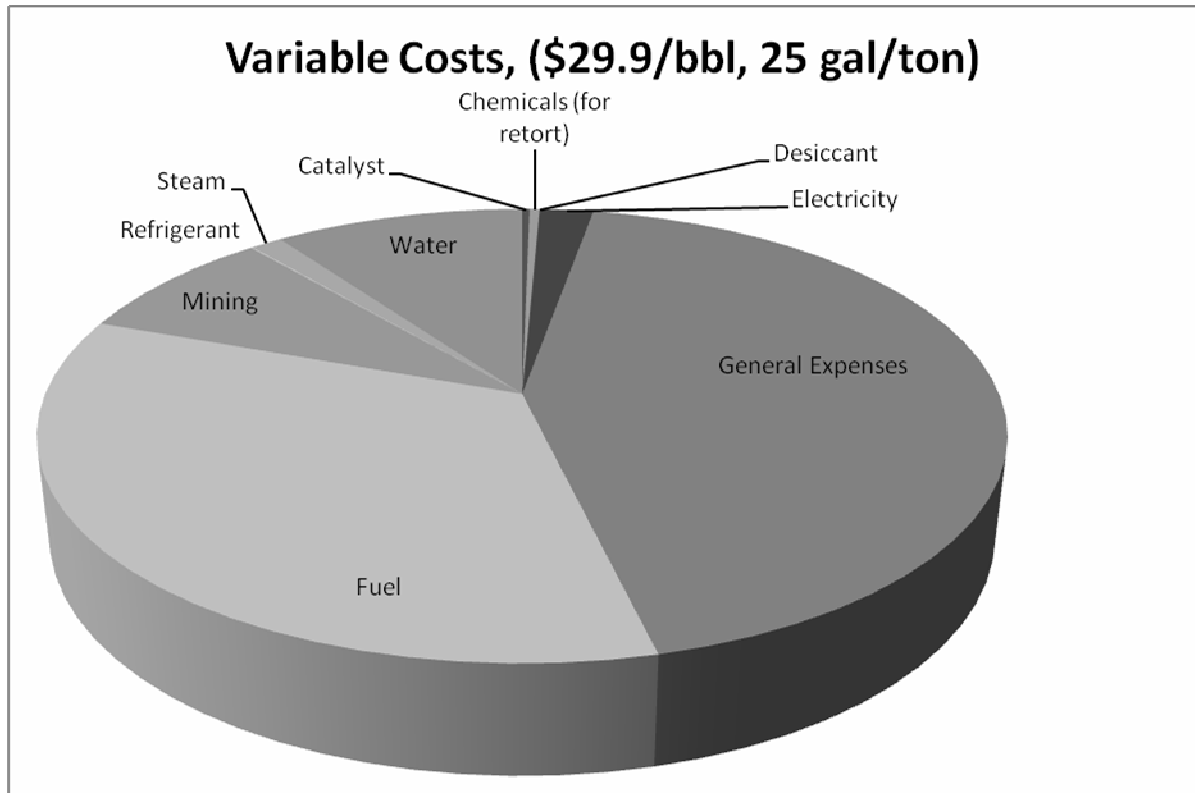


Figure 4.3: Air-fired Variable Costs Distribution for the 25 Gal/ton Case

Table 4.2: Variable Costs (\$/bbl) for the 25 Gal/ton Case

Catalyst	0.088722787	0.30%
Chemicals (for retort)	0.11618298	0.39%
Desiccant	0.005147019	0.02%
Electricity	0.63539119	2.13%
General Expenses	12.97156588	43.41%
Fuel	10.24745691	34.29%
Mining	2.455827766	8.22%
Refrigerant	0.019035786	0.06%
Steam	0.3741696	1.25%
Water	2.966986593	9.93%
Total	29.88048651	100.00%

The base case scenario revealed a cost of \$112/bbl, with a return on investment (ROI) of 18% and a payback period of 3.56 years. Returning to Figure 4.2, we can see the impact of the oil shale grade on the supply costs. As the oil shale grade goes down to 20 gal/ton and up to 35 gal/ton, the supply costs increase to \$124/bbl and decrease to \$97/bbl, respectively.

Tax on CO₂ increases the base case scenario supply cost by 1.75% or \$114.65/bbl. This increase is reflected in a 3.7% increase in the total annual operating costs, which is \$1,022 million.

4.2 Oxy-fired Case

4.2.1 Capital Costs

Using the same average mined oil shale grade of 25 gal/ton as in the air-fired case, but with an oxy-fired combustion for plant heating requirements and compression and sales of CO₂ for EOR or other sequestration, the Base *Ex Situ* Case was developed.

The total depreciable capital for this plant is \$3.39 Billion. The capital costs are categorized as retorting and mining (70.8%), hydrotreater (23%), water reservoir (11%) and oil pipeline (3.3%), in that order. The CO₂ compression plant and hydrogen plant are much smaller, corresponding to 0.96% and 0.29% respectively. Note that for the air case, there was not a CO₂ compression plant. The relative capital expenditures are summarized in Figure 4.4. Table 4.3 contains the costs for each part of the process.

The variation of oil shale grade again shows higher capital costs for the lower grade cases and vice versa: \$3.69 and \$3.00 billion for the 20 gal/ton and 35 gal/ton case, respectively.

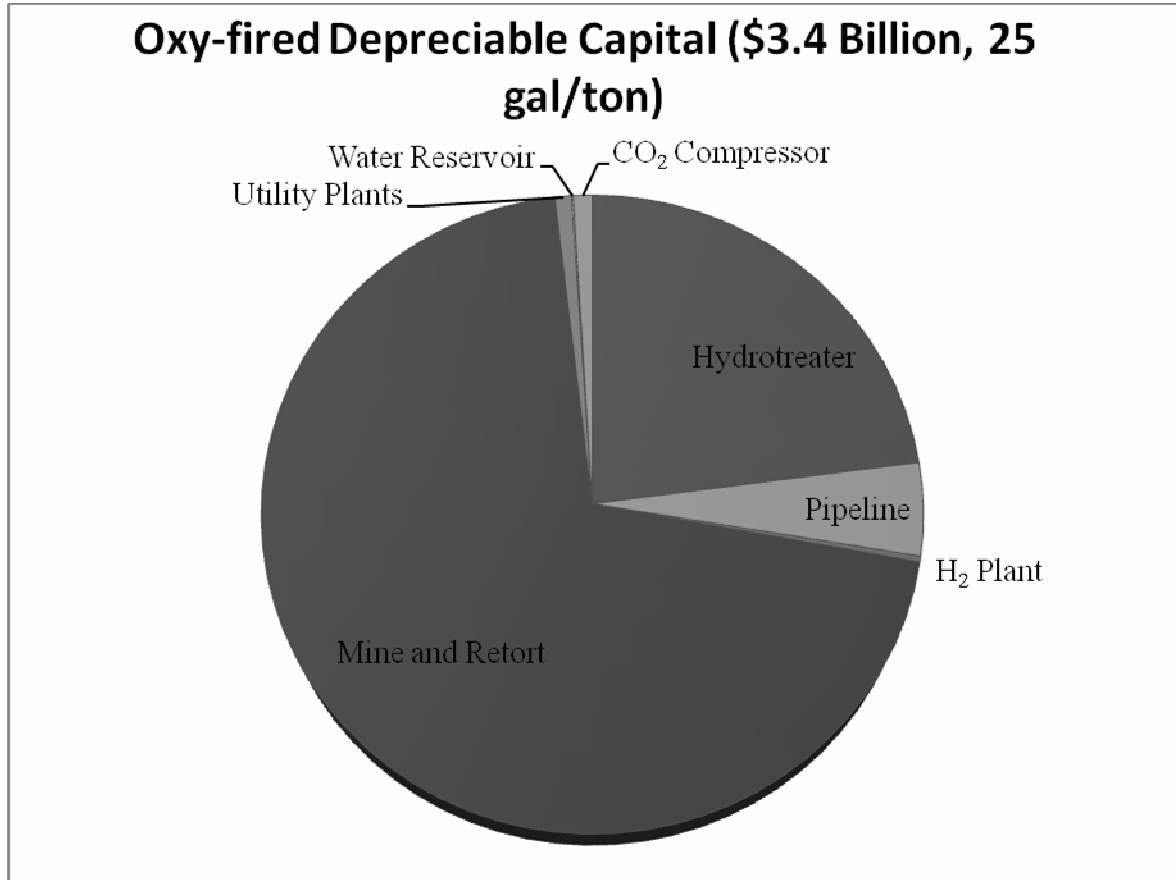


Figure 4.4: Pie Chart of Capital Costs for *Ex Situ* Oil Shale Extraction and Upgrading for Oxy-Fired Plant Heat Requirements

Table 4.3: Oxy-Fired Process Total Depreciable Capital

Hydrotreater	\$ 727,324,018.44	23.11%
Pipeline	\$ 148,923,634.96	4.73%
H ₂ Plant	\$ 9,116,149.51	0.29%
Mine and Retort	\$ 2,229,060,359.91	70.82%
Utility Plants	\$ 26,536,602.76	0.84%
Water Reservoir	\$ 2,582,680.08	0.08%
CO ₂ Compressor	\$ 30,301,681.09	0.96%
Subtotal	\$ 3,147,308,523.99	100.00%
Total	\$ 3,391,571,793.51	

4.2.2 Annual Sales and Costs

The total annual operating costs for this case were calculated to be \$1,160 million with \$445 million corresponding to fixed costs and \$715 million in variable costs. Among these annual costs, the highest costs are labor (32%), fuel (26%) and general expenses (22%). Moreover, oxygen had to be included as a new utility cost; it consisted of 10.8% of the total annual costs.

Again, to provide a sensitivity analysis for the oil shale grade, revenues for the base case and its variants are presented in Figure 4.5. In the top C-Base bar from the base scenario we find that the largest costs for Profit (ROI) which consists of \$39.4/bbl are the variable annual costs, followed by earnings \$32/bbl and taxes \$17/bbl. While the annual fixed costs corresponded to \$10.78/bbl and a total depreciable capital of \$11.27/bbl, the revenue due to selling CO₂ turned out to be \$1.8/bbl. The biggest subcategories within the variable cost were the general expenses (36.3 %) and fuel (25.9%). For this base case, these costs were broken into percentages of the total variable cost, as shown in Figure 4.6 and Table 4.4.

The base case scenario revealed a cost of \$122/bbl, with a return on investment (ROI) of 18% and a payback period of 3.59 years. The impact of the oil shale grade on the supply costs are presented in this case too. As the oil shale grade goes down to 20 gal/ton and up to 30 and 35 gal/ton, the supply costs increased to \$135/bbl and decreased to \$112/bbl and \$105/bbl, respectively.

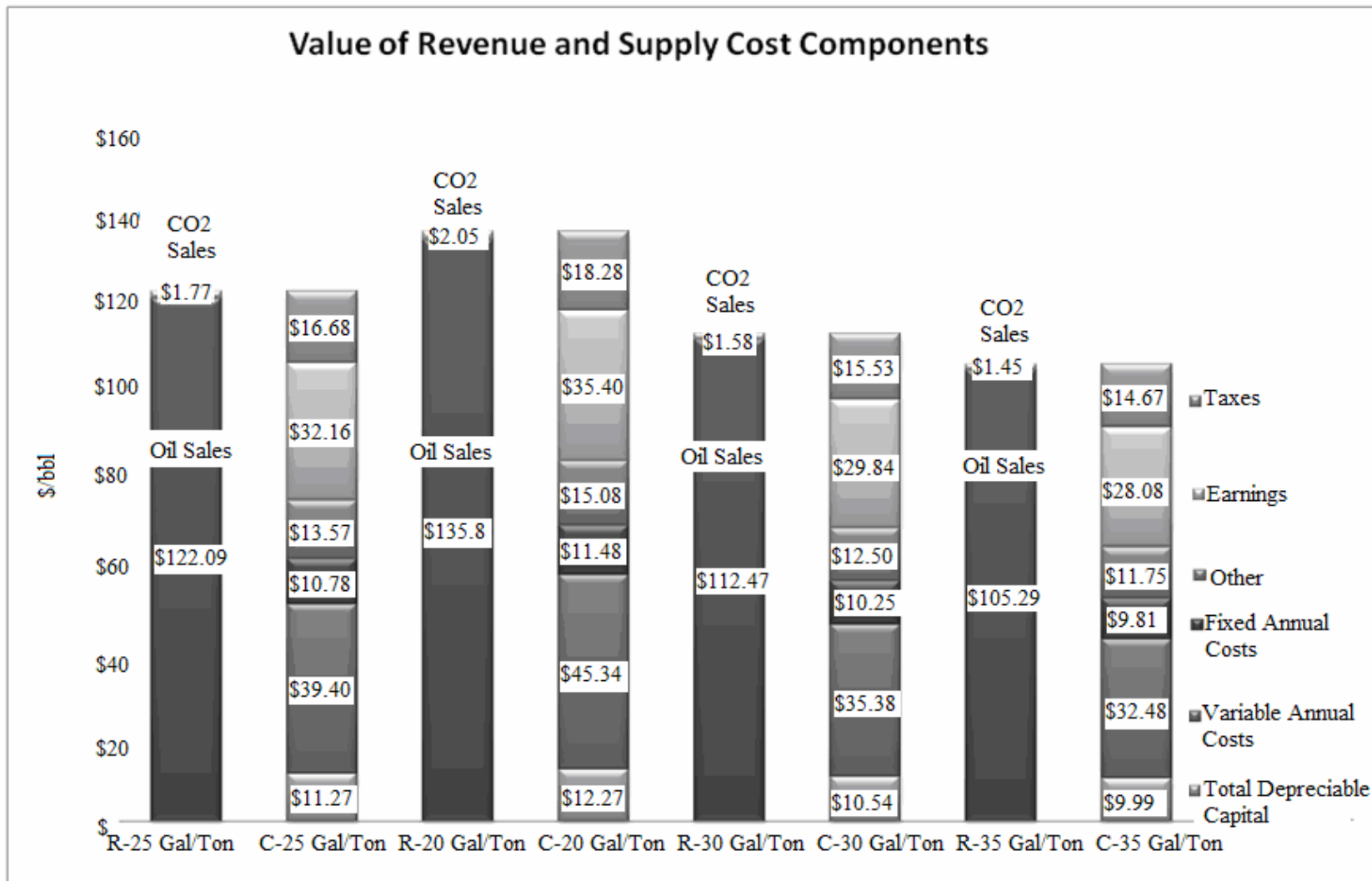


Figure 4.5: Revenue and Cost of *Ex Situ* Oil Shale Extraction and Upgrading for Oxy-Fired Plant Heat Requirements—Variable Grade of Oil Shale

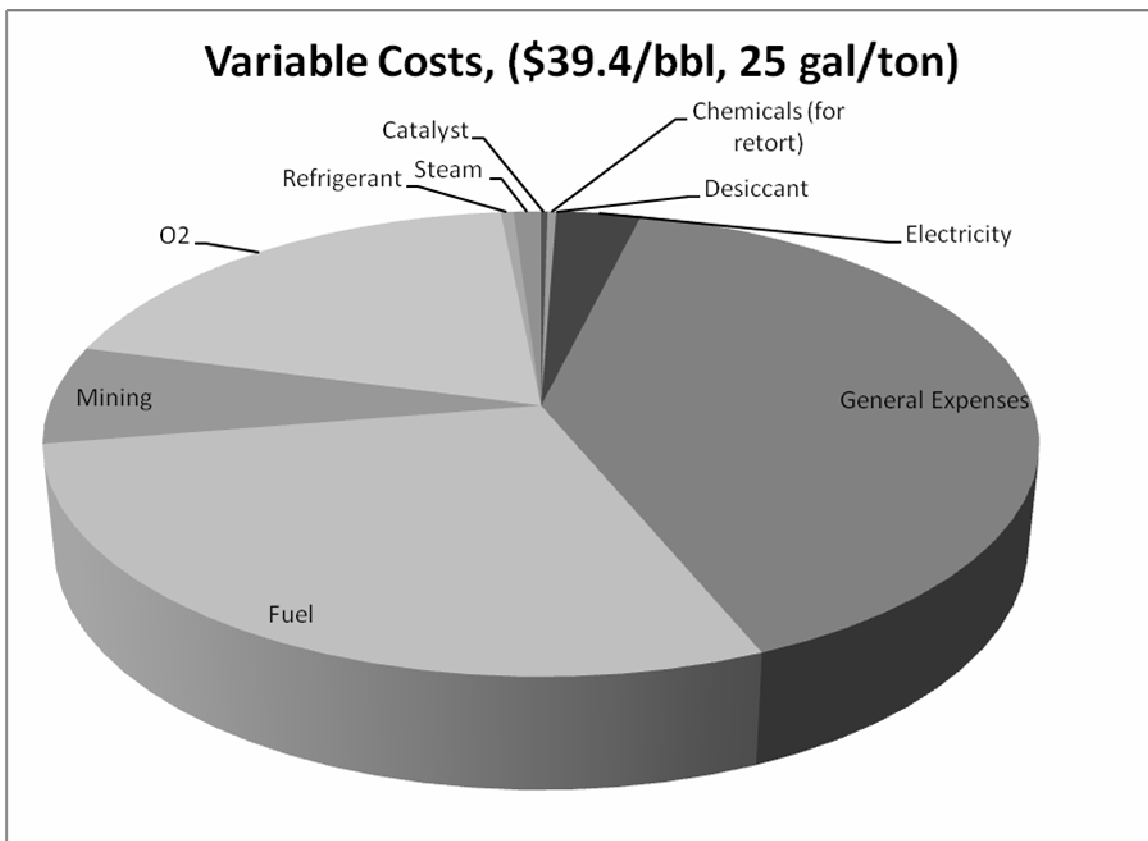


Figure 4.6: Oxy-fired Variable Costs Distribution for the 25 Gal/ton Base Case

Table 4.4: Variable Costs (\$/bbl) for the 25 Gal/ton Case

Catalyst	0.088729009	0.23%
Chemicals (for retort)	0.11618298	0.29%
Desiccant	0.005145813	0.01%
Electricity	1.147805834	2.91%
General Expenses	14.30548136	36.31%
Fuel	10.22430808	25.95%
Mining	2.455827766	6.23%
O2	6.8825931	17.47%
Refrigerant	0.172320189	0.44%
Steam	0.3741696	0.95%
Water	3.62707739	9.21%
Total	39.39964112	100.00%

4.3 Oxy vs. Air-Fired Burners

The presented results clearly show that oxy-fired burners with a CO₂ compression system entail high costs. For a base case scenario of 25 gal/ton without CO₂ taxation, the cost for an air-fired process was \$112/bbl while the cost of the oxy-fired case was \$122/bbl. The cost increase for compressing and selling CO₂ is 8.2% which is higher than the 1.75% increase due to taxation.

CHAPTER 5

OTHER IMPORTANT CONSIDERATIONS

5.1 Safety and Process Control

A further step that should be taken before moving to final implementation of the proposed design is completion of a hazard and operability (HAZOP) study in accordance with the AIChE Center for Chemical Process Safety guidelines (AIChE, 1993). However, a preliminary safety assessment reveals the following potential safety issues:

- Extreme temperatures and pressures in process equipment and streams.
- Control of exothermic reactors.
- Health hazards associated with some reactants and products.
- Flammability of reactants and products.

Therefore, even without the specific findings of a HAZOP study, it is clear that certain safety features will be required. All process equipment will require temperature and pressure and capacity alarms. Exothermic reactors should be paired with automatic safety interlock systems to prevent run-away reactions. Pressure vessels will require rupture disks and safety valves that lead to either blow-down tanks or a flare. Air monitoring equipment should be installed to alert personnel to dangerous levels of pollutants. The plant should limit its inventory of flammable material to only what is absolutely necessary and isolate potential fuels from oxidizers.

5.2 Environmental Issues

Since the project was meant to be developed in the Utah, a study of the environmental regulations to be followed is required. There are different situations that required a detailed analysis such as the following:

- Burning fossil fuels for power generation: Effluent gases from burners and fires usually consist of NO_x, CO₂, CO, soot and ash which produce the so-called greenhouse gases, volatile toxic compounds, acid rains and others. For that reason, it is recommended to consider separating sulfur, nitrogen and other components from fuels or effluent gases.
- Handling toxic wastes: During the process design of the plant, facilities to remove pollutants from water and waste materials have to be included.
- Bioaccumulated chemicals
- Toxic metals and minerals: During the upgrading of oil, it releases metals which are potential hazards such as mercury, lead, cadmium and others. Techniques to dispose and handle them have to be evaluated and implemented.

Finally, since it is expected that new plants will have to meet higher environmental standards, it is necessary to plan for the following:

- Reducing and Reusing Wastes
- Avoiding Nonroutine Events
- Reaction Pathways to Reduce Byproduct Toxicity

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

This project studied the production of oil shale at a scale of 50,000 bbl/d. The oil shale process involved mining, an *ex situ* retort, a hydrotreater and a pipeline for delivery. In addition, oxy-fired and air-fired burners were considered as technological variations. After the process design, engineering costing methods were used to obtain equipment costs as well as utilities, enabling the economical study. The economical analysis consisted of quantifying all costs of production and revenue on \$/bbl basis, identifying market conditions under which the process breaks even and performing a sensitivity of the process.

This project revealed that the total capital invested to develop oil shale projects is enormous. At a richness of 25 gal/ton basis, the total depreciable capital was of \$3.34 and \$3.39 billion for the air and the oxy-fired cases, respectively. It is evident that oil shale projects require significantly higher investments than conventional oil (which are already very capital intensive) and contain both technical and economic risks that conventional oil projects do not.

Oil shale economics fluctuate broadly depending on the quality or richness of the resource, the technology used (e.g. CO₂ compression) and taxation of CO₂ emissions. For different resource grades, the supply cost varied. For shale grades of 20, 25 and 35

gal/ton, the supply cost varied from \$124/bbl, \$112/bbl and \$97/bbl, respectively. Moreover, this study showed that the oil shale project profitability is highly dependent on governmental policies. The potential taxation of CO₂ increased the supply cost by 1.75% above the air-base case to \$120/bbl from \$112/bbl. In addition, it was shown that the highest variable costs turned out to be the sales expenses, direct research, allocated research, administrative expenses and management incentives, followed by the fuel in both air and oxy-fired cases.

From these results, it can be concluded that oil shale projects have higher technical, economic and government policy risks which limit their use by industry. For more projects to move forward, these risks must be lowered. It is also clear from the supply cost analysis that royalties are a major component as are taxes and interest charges.

It is recommended to perform a sensitivity analysis on each of the variable costs, as well as the scale of the process. These variations will help to fully understand their impact on the supply cost of oil. For further studies, *in situ* technologies must be considered as a potential alternative.

APPENDIX

A-1 Kinetic Rate Constants for Upgrader

Table A-1 Kinetic Rate Constants

Kinetic constant (h ⁻¹)	Temperature 788°F	Activation Energy (kcal/mol)
K1	0.362	48.5
K2	0.057	44.2
K3	0.043	38.0
K4	0.137	27.3
K5	0.104	39.5
K6	0.016	37.1
K7	0	
K8	0.01	53.7
K9	0	
K10	0	
k _{sulfur}	10.46 @693.15 K	136.23
K _{nitrogen}	2.437 @693.15 K	97.99

A-2 Air-fired Combustor

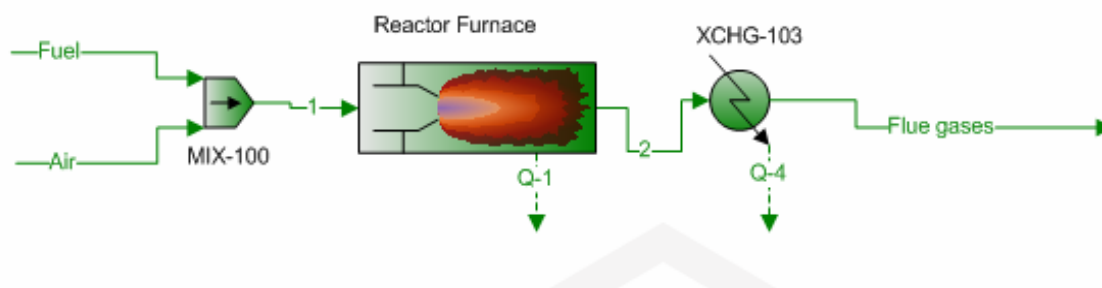


Figure A-1 Schematic of an Air-Fired Burner

Table A-2 Air-fired Burner Stream Composition

Stream		Fuel	Air	1
Temperature	°F	674	674	673.99
Pressure	Atm	1	1	1
Mole Fraction Vapor	%	100	100	100
Molecular Weight	lb/lbmol	16.04	29.09	27.71
Mass Density	lb/ft ³	0.02	0.04	0.03
Molar Flow	lbmol/h	1,387.80	11,758.00	13,145.80
Mass Flow	lb/h	22,263.73	342,062.61	364,326.33
Vapor Volumetric Flow	ft ³ /h	1,149,159.03	9,737,689.83	10,886,878.15
Liquid Volumetric Flow	Gpm	143,271.78	1,214,049.64	1,357,325.07
Std Vapor Volumetric Flow	MMSCFD	12.64	107.09	119.73
Std Liquid Volumetric Flow	Sgpm	148.42	777.22	925.64
Species flow rate	lb/h			
Oxygen		0	88,822.74	88,822.74
Methane		22,263.73	0	22,263.73
Carbon Dioxide		0	0	0
Water		0	0	0
Nitrogen			247,822.96	247,822.96
Argon			5,416.90	5,416.90

Table A-2 Continued

Stream	2	Flue gases
Temperature	4,247.06	650
Pressure	1	9.7
Mole Fraction Vapor	100	100
Molecular Weight	27.71	27.71
Mass Density	0.01	0.02
Molar Flow	13,145.80	13,145.80
Mass Flow	364,326.33	364,326.33
Vapor Volumetric Flow	45,187,428.27	16,147,316.31
Liquid Volumetric Flow	5,633,757.29	2,013,171.90
Std Vapor Volumetric Flow	119.73	119.73
Std Liquid Volumetric Flow	870.28	870.28
Species flow rate		
Oxygen	6.87	6.87
Methane	0	0
Carbon Dioxide	61,076.38	61,076.38
Water	50,003.21	50,003.21
Nitrogen	247,822.96	247,822.96
Argon	5,416.90	5,416.90

A-3 Oxy-fired Combustor

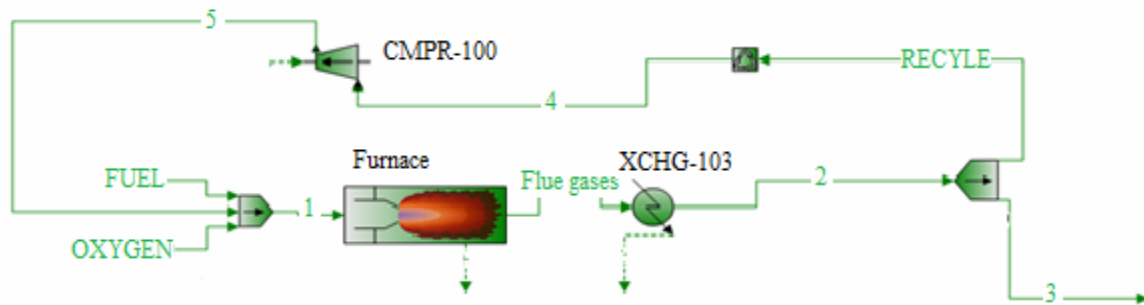


Figure A-3 Schematic of an Air-Fired Burner

Table A-3 Oxy-fired Combustor Stream Composition

Stream		Fuel	Oxygen	1
Temperature	°F	674	674	726.18
Pressure	Atm	1	1	1
Mole Fraction Vapor	%	100	100	100
Molecular Weight	lb/lbmol	16.04	32	26.68
Mass Density	lb/ft ³	0.02	0.04	0.03
Molar Flow	lbmol/h	1,373.20	2,750.00	10,307.70
Mass Flow	lb/h	22,029.51	87,996.70	275,060.70
Vapor Volumetric Flow	ft ³ /h	1,137,069.60	2,277,248.43	8,924,624.41
Liquid Volumetric Flow	Gpm	141,764.52	283,916.69	1,112,680.45
Std Vapor Volumetric Flow	MMSCFD	12.51	25.05	93.88
Std Liquid Volumetric Flow	Sgpm	146.86	154	669.96
Species flow rate	lb/h			
Oxygen		0	87,996.70	88,188.70
Methane		22,029.51	0	22,029.51
Carbon Dioxide		0	0	90,637.56
Water		0	0	74,204.93

Table A-3 Continued

Stream		Flue gases	2	3
Temperature	°F	4,224.37	650	650
Pressure	Atm	1	0.66	0.66
Mole Fraction Vapor	%	100	100	100
Molecular Weight	lb/lbmol	26.68	26.68	26.68
Mass Density	lb/ft ³	0.01	0.02	0.02
Molar Flow	lbmol/h	10,307.70	10,307.70	4,123.08
Mass Flow	lb/h	275,060.70	275,060.70	110,024.28
Vapor Volumetric Flow	ft ³ /h	35,259,463.56	12,650,869.43	5,060,347.77
Liquid Volumetric Flow	Gpm	4,395,985.07	1,577,251.25	630,900.50
Std Vapor Volumetric Flow	MMSCFD	93.88	93.88	37.55
Std Liquid Volumetric Flow	Sgpm	615.18	615.18	246.07
Species flow rate	lb/h			
Oxygen		307.2	307.2	122.88
Methane		0	0	0
Carbon Dioxide		151,071.41	151,041.41	60,428.56
Water		123,682.10	123,682.10	49,472.84

Table A-3 Continued

Stream		recycle	4	5
Temperature	°F	650.00	650.00	760.29
Pressure	Atm	0.66	0.66	1.00
Mole Fraction Vapor	%	100.00	100.00	100.00
Molecular Weight	lb/lbmol	26.68	26.68	26.69
Mass Density	lb/ft ³	0.02	0.02	0.03
Molar Flow	lbmol/h	6,184.62	6,184.62	6,184.50
Mass Flow	lb/h	165,036.42	165,036.42	165,034.50
Vapor Volumetric Flow	ft ³ /h	7,590,521.66	7,590,521.66	5,505,557.09
Liquid Volumetric Flow	Gpm	946,350.75	946,350.75	686,407.12
Std Vapor Volumetric Flow	MMSCFD	56.33	56.33	56.33
Std Liquid Volumetric Flow	Sgpm	369.11	369.11	369.10
Species flow rate	lb/h			
Oxygen		184.32	184.32	184.32
Methane		0.00	0.00	0.00
Carbon Dioxide		90,642.84	90,642.84	90,642.84
Water		74,209.26	74,209.26	74,209.26

A-4 Naphtha Hydrotreater

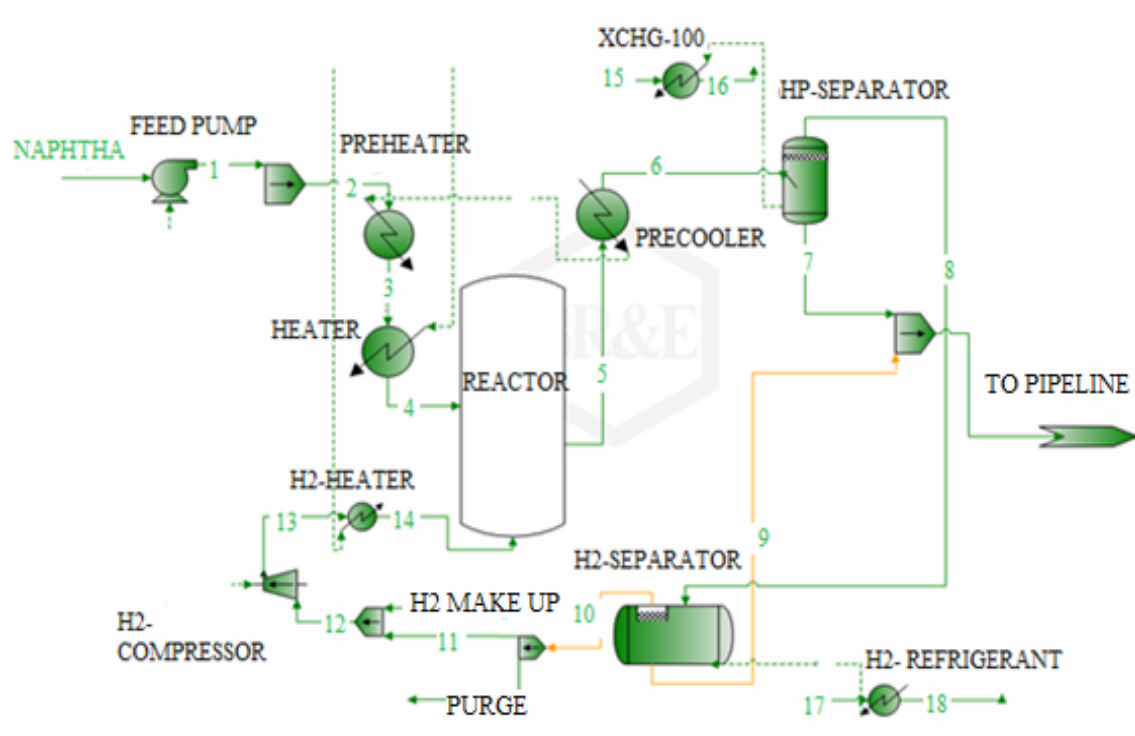


Figure A-4 Naphtha Hydrotreater Schematic

Table A-4 Naphtha Hydrotreater Stream Composition

Stream		Naphtha	1	2
Temperature	°F	68	71.93	71.93
Pressure	Atm	1	86.85	86.85
Mole Fraction Vapor	%	0	0	0
Mole Fraction Light Liquid	%	100	100	100
Mole Fraction Heavy Liquid	%	0	0	0
Molecular Weight	lb/lbmol	107.51	107.51	107.51
Mass Density	lb/ft ³	770,918.86	48.58	48.58
Molar Flow	lbmol/h	829.68	829.68	829.68
Mass Flow	lb/h	89,199.14	89,199.14	89,199.14
Vapor Volumetric Flow	ft ³ /h	1,853.42	1,836.30	1,836.30
Liquid Volumetric Flow	gpm	231.57	228.94	228.94
Std Vapor Volumetric Flow	MMSCFD	7.56	7.56	7.56
Std Liquid Volumetric Flow	sgpm	229.98	229.98	229.98
Species flow rate	lb/h			
Naphtha		89,199.14	89,199.14	89,199.14
Hydrogen		0	0	0
NH3		0	0	0
Hydrogen Sulfide		0	0	0

Table A-4 Continued

Stream		3	4	5
Temperature	°F	392	842	803.71
Pressure	Atm	86.71	86.58	85.86
Mole Fraction Vapor	%	0	100	100
Mole Fraction Light Liquid	%	100	0	0
Mole Fraction Heavy Liquid	%	0	0	0
Molecular Weight	lb/lbmol	107.51	107.51	27.6
Mass Density	lb/ft ³	38.4	14.63	2.51
Molar Flow	lbmol/h	829.68	829.68	3,414.31
Mass Flow	lb/h	89,199.14	89,199.14	94,224.65
Vapor Volumetric Flow	ft ³ /h	2,323.04	6,095.23	37,511.37
Liquid Volumetric Flow	gpm	289.63	759.92	4,676.74
Std Vapor Volumetric Flow	MMSCFD	7.56	7.56	31.1
Std Liquid Volumetric Flow	sgpm	229.98	229.98	372.75
Species flow rate	lb/h			
Naphtha		89,199.14	89,199.14	86,978.09
Hydrogen		0	0	5,025.51
NH3		0	0	1,605.58
Hydrogen Sulfide		0	0	615.47

Table A-4 Continued

Stream		6	7	8	9
Temperature	°F	607.2	122	122	32
Pressure	atm	85.73	84.37	84.37	83
Mole Fraction Vapor	%	100	0	100	0
Mole Fraction Light Liquid	%	0	100	0	100
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	27.6	98.11	2.53	86.99
Mass Density	lb/ft ³	3.01	46.94	0.48	50.49
Molar Flow	lbmol/h	3,414.31	895.41	2,518.90	4.17
Mass Flow	lb/h	94,224.65	87,852.33	6,372.33	362.87
Vapor Volumetric Flow	ft ³ /h	31,298.45	1,871.42	13,295.00	7.19
Liquid Volumetric Flow	gpm	3,902.14	233.32	1,657.56	0.9
Std Vapor Volumetric Flow	MMSCFD	31.1	8.16	22.94	0.04
Std Liquid Volumetric Flow	sgpm	372.75	228.55	144.2	0.95
Species flow rate	lb/h				
Naphtha		86,978.09	86,605.02	373.07	346.24
Hydrogen		5,025.51	57.96	4,967.55	0.18
NH ₃		1,605.58	892.3	713.28	12.9
Hydrogen Sulfide		615.47	297.04	318.43	3.55

Table A-4 Continued

Stream		13	14	15
Temperature	°F	456.91	842	68
Pressure	atm	86.85	86.51	1.36
Mole Fraction Vapor	%	100	100	0
Mole Fraction Light Liquid	%	0	0	100
Mole Fraction Heavy Liquid	%	0	0	0
Molecular Weight	lb/lbmol	2.31	2.31	18.02
Mass Density	lb/ft ³	0.29	0.2	62.29
Molar Flow	lbmol/h	3,140.01	3,140.01	46,352.05
Mass Flow	lb/h	7,241.73	7,241.73	835,045.08
Vapor Volumetric Flow	ft ³ /h	25,020.22	35,335.81	13,404.72
Liquid Volumetric Flow	gpm	3,119.40	4,405.50	1,671.24
Std Vapor Volumetric Flow	MMSCFD	28.6	28.6	422.16
Std Liquid Volumetric Flow	sgpm	178.8	178.8	1,669.32
Species flow rate	lb/h			
Naphtha		26.025296	26.0253	0
Hydrogen		6230.9049	6230.905	0
NH3		679.37156	679.3716	0
Hydrogen Sulfide		305.43236	305.4324	0
R-134a		0	0	0
Water				835,045.08

Table A-4 Continued

Stream		16	17	18
Temperature	°F	120	-151.6	-98
Pressure	atm	1.22	1.7	1.565057
Mole Fraction Vapor	%	0	0	0
Mole Fraction Light Liquid	%	100	100	100
Mole Fraction Heavy Liquid	%	0	0	0
Molecular Weight	lb/lbmol	18.02	102.03	102.03
Mass Density	lb/ft ³	61.67	103.4	98.53
Molar Flow	lbmol/h	46,352.05	1,149.64	1149.63
Mass Flow	lb/h	835,045.08	117,298.71	117298.7
Vapor Volumetric Flow	ft ³ /h	13,540.72	1,134.37	1190.4
Liquid Volumetric Flow	gpm	1,688.19	141.43	148.41
Std Vapor Volumetric Flow	MMSCFD	422.16	10.47	10.47
Std Liquid Volumetric Flow	sgpm	1,669.32	188.94	188.93
Species flow rate	lb/h			
Naphtha		0	0	0
Hydrogen		0	0	0
NH3		0	0	0
Hydrogen Sulfide		0	0	0
R-134a		0	117298.7	117298.7
Water		835,045.08	0	0

A-5 Distillates Hydrotreater

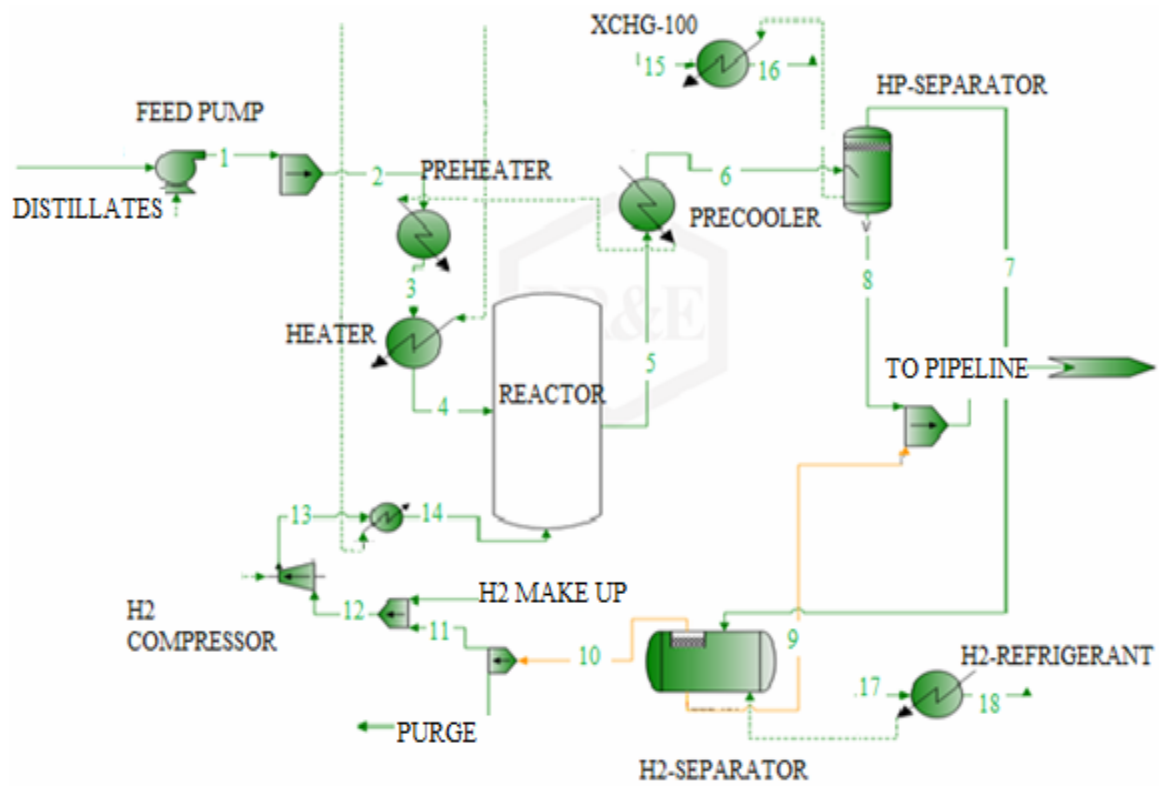


Figure A-5 Distillates Hydrotreater Schematic

Table A-5 Distillates Hydrotreater Stream Composition

Stream		Distillates	1	2
Temperature	°F	68	68	68
Pressure	atm	1	86.85	86.85
Mole Fraction Light Liquid	%	100	100	100
Molecular Weight	lb/lbmol	231.71	231.71	231.71
Mass Density	lb/ft ³	58.06	58.06	58.06
Molar Flow	lbmol/h	1,636.71	1,636.71	1,636.71
Mass Flow	lb/h	379,239.23	379,239.23	379,239.23
Vapor Volumetric Flow	ft ³ /h	6,531.84	6,531.84	6,531.84
Liquid Volumetric Flow	gpm	816.11	816.11	816.11
Std Vapor Volumetric Flow	MMSCFD	14.91	14.91	14.91
Std Liquid Volumetric Flow	sgpm	811.68	811.68	811.68
Species flow rate	lb/h			
Gas Oil		379,239.23	379,239.23	379,239.23

Table A-5 Continued

Stream		3	4
Temperature	°F	392	842
Pressure	atm	86.71	86.58
Mole Fraction Light Liquid	%	100	100
Molecular Weight	lb/lbmol	231.71	231.71
Mass Density	lb/ft ³	50.27	36.78
Molar Flow	lbmol/h	1,636.71	1,636.71
Mass Flow	lb/h	379,239.23	379,239.23
Vapor Volumetric Flow	ft ³ /h	7,544.05	10,310.97
Liquid Volumetric Flow	gpm	940.56	1,285.52
Std Vapor Volumetric Flow	MMSCFD	14.91	14.91
Std Liquid Volumetric Flow	sgpm	811.68	811.68
Species flow rate	lb/h		
Gas Oil		379,239.23	379,239.23

Table A-5 Continued

Stream		5	6	7	8
Temperature	°F	779.87	634.42	122	122
Pressure	atm	86.85	86.71	85.35	85.35
Mole Fraction Vapor	%	98.76	89.77	100	0
Mole Fraction Light Liquid	%	1.24	10.23	0	100
Molecular Weight	lb/lbmol	34.36	34.36	2.59	135.86
Mass Density	lb/ft ³	3.26	3.83	0.5	52.27
Molar Flow	lbmol/h	11,542.52	11,542.52	8,790.36	2,752.16
Mass Flow	lb/h	396,647	396,647.00	22,749.01	373,897.99
Vapor Volumetric Flow	ft ³ /h	121,702.	103,477.85	45,864.09	7,153.27
Liquid Volumetric Flow	gpm	15,173.24	12,901.13	5,718.12	891.84
Std Vapor Volumetric Flow	MMSCFD	105.12	105.12	80.06	25.07
Std Liquid Volumetric Flow	sgpm	1,384.40	1,384.40	502.44	881.95
Species flow rate	lb/h				
Gas Oil		202,587.9	202,587.9	0.02	202,587.9
Hydrogen		17,407.77	17,407.77	17,235.	172.76
NH ₃		6,826.31	6,826.31	3,250.10	3,576.21
Hydrogen Sulfide		2,616.75	2,616.75	1,439.22	1,177.53
Naphtha		167,208.	167,208.	824.65	166,383.

Table A-5 Continued

Stream		9	10	Purge	11
Temperature	°F	121.96	32	32	32
Pressure	atm	83.99	83.99	83.99	83.99
Mole Fraction Vapor	%	0.05	100	100	100
Mole Fraction Light Liquid	%	99.95	0	0	0
Molecular Weight	lb/lbmol	135.66	2.5	2.5	2.5
Mass Density	lb/ft ³	52.21	0.56	0.56	0.56
Molar Flow	lbmol/h	2,761.89	8,780.64	263.42	8,517.22
Mass Flow	lb/h	374,686.18	21,960.82	658.82	21,302.00
Vapor Volumetric Flow	ft ³ /h	7,176.53	39,528.71	1,185.86	38,342.85
Liquid Volumetric Flow	gpm	894.74	4,928.26	147.85	4,780.41
Std Vapor Volumetric Flow	MMSCFD	25.15	79.97	2.4	77.57
Std Liquid Volumetric Flow	sgpm	884.02	500.37	15.01	485.36
Species flow rate	lb/h				
Gas Oil		202,587.95	0	0	0
Hydrogen		173.17	17,234.60	517.04	16,717.56
NH ₃		3,616.26	3,210.06	96.3	3,113.76
Hydrogen Sulfide		1,188.38	1,428.37	42.85	1,385.52
Naphtha		167,120.42	87.79	2.63	85.16

Table A-5 Continued

Stream		H2 Makeup	12
Temperature	°F	100	50.27
Pressure	atm	13.61	13.61
Mole Fraction Vapor	%	100	100
Molecular Weight	lb/lbmol	2.02	2.39
Mass Density	lb/ft ³	0.07	0.09
Molar Flow	lbmol/h	2,600.78	11,118.00
Mass Flow	lb/h	5,242.87	26,544.87
Vapor Volumetric Flow	ft ³ /h	78,738.85	306,737.81
Liquid Volumetric Flow	gpm	9,816.79	38,242.64
Std Vapor Volumetric Flow	MMSCFD	23.69	101.26
Std Liquid Volumetric Flow	sgpm	147.9	633.26
Species flow rate	lb/h		
Hydrogen		5,242.87	21,960.43
NH3		0	3,113.76
Hydrogen Sulfide		0	1,385.52
Naphtha		0	85.16

Table A-5 Continued

Stream		13	14	15
Temperature	°F	456.99	842	68
Pressure	atm	86.85	86.51	1.36
Mole Fraction Vapor	%	100	100	0
Mole Fraction Light Liquid	%	0	0	100
Molecular Weight	lb/lbmol	2.39	2.39	18.02
Mass Density	lb/ft ³	0.3	0.21	62.29
Molar Flow	lbmol/h	11,118.00	11,118.00	176,764.75
Mass Flow	lb/h	26,544.87	26,544.87	3,184,466.48
Vapor Volumetric Flow	ft ³ /h	88,595.45	125,118.13	51,119.24
Liquid Volumetric Flow	gpm	11,045.67	15,599.14	6,373.31
Std Vapor Volumetric Flow	MMSCFD	101.26	101.26	1,609.91
Std Liquid Volumetric Flow	sgpm	633.26	633.26	6,365.98
Species flow rate	lb/h			
Hydrogen		21,960.43	21,960.43	0
NH ₃		3,113.76	3,113.76	0
Hydrogen Sulfide		1,385.52	1,385.52	0
R-134a		0	0	0
Water		0	0	3,184,466.48
Naphtha		85.16	85.16	0

Table A-5 Continued

Stream		16	17	18
Temperature	°F	120	-151.6	-144.4
Pressure	atm	1.22	1.7	1.57
Mole Fraction Vapor	%	0	0	0
Mole Fraction Light Liquid	%	100	100	100
Molecular Weight	lb/lbmol	18.02	102.03	102.03
Mass Density	lb/ft ³	61.67	103.4	102.76
Molar Flow	lbmol/h	176,764.75	30,286.12	30,286.12
Mass Flow	lb/h	3,184,466.48	3,090,119.85	3,090,119.85
Vapor Volumetric Flow	ft ³ /h	51,637.91	29,883.82	30,070.30
Liquid Volumetric Flow	gpm	6,437.97	3,725.77	3,749.02
Std Vapor Volumetric Flow	MMSCFD	1,609.91	275.83	275.83
Std Liquid Volumetric Flow	sgpm	6,365.98	4,977.34	4,977.34
Species flow rate	lb/h			
Hydrogen		0	0	0
NH ₃		0	0	0
Hydrogen Sulfide		0	0	0
R-134a		0	3,090,119.85	3,090,119.85
Water		3,184,466.48	0	0
Naphtha		0	0	0

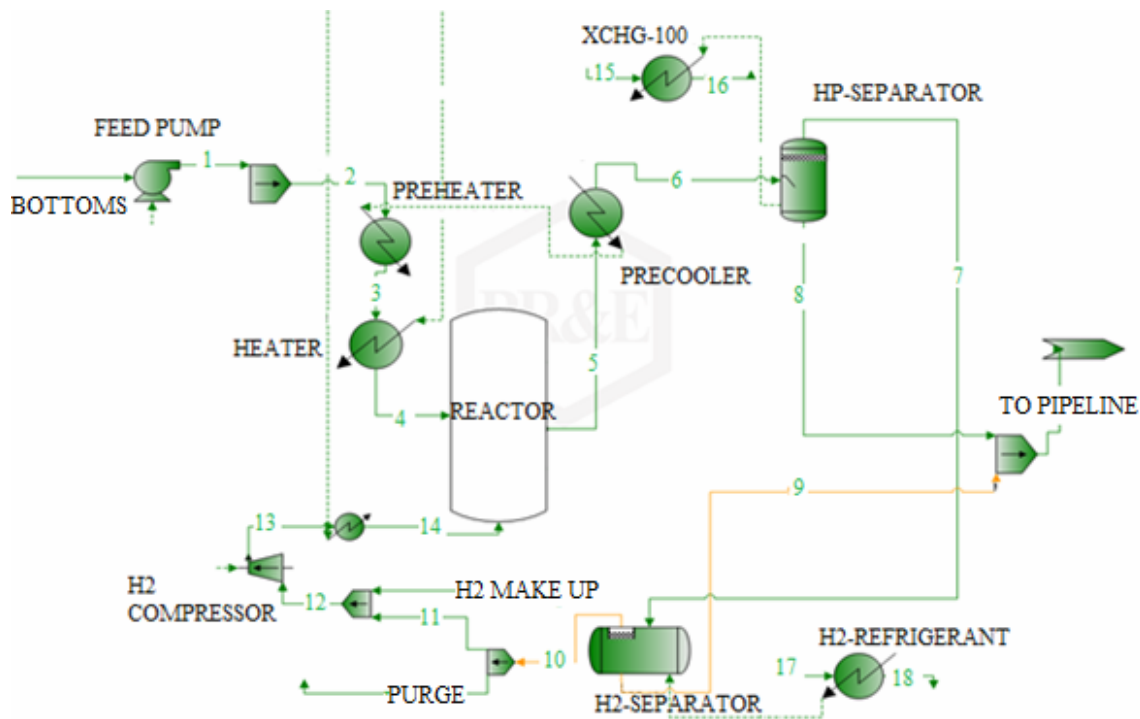
A-6 Bottoms Hydrotreater

Figure A-6 Bottoms Hydrotreater Schematic

Table A-6 Bottoms Hydrotreater Stream Composition

Stream		Bottoms	1	2
Temperature	°F	68	65.41	65.41
Pressure	atm	1	86.85	86.85
Mole Fraction Light Liquid	%	100	100	100
Molecular Weight	lb/lbmol	420.07	420.07	420.07
Mass Density	lb/ft ³	63.76	64.02	64.02
Molar Flow	lbmol/h	379.93	379.93	379.93
Mass Flow	lb/h	159,596.51	159,596.51	159,596.51
Vapor Volumetric Flow	ft ³ /h	2,503.04	2,492.83	2,492.83
Liquid Volumetric Flow	gpm	312.74	310.79	310.79
Std Vapor Volumetric Flow	MMSCFD	3.46	3.46	3.46
Std Liquid Volumetric Flow	sgpm	311.14	311.14	311.14
Species flow rate	lb/h			
Bottoms		159,596.51	159,596.51	159,596.51

Table A-6 Continued

Stream		3	4
Temperature	°F	392	842
Pressure	atm	1,274.33	86.58
Mole Fraction Light Liquid	%	100	100
Molecular Weight	lb/lbmol	420.07	420.07
Mass Density	lb/ft ³	56.13	44.56
Molar Flow	lbmol/h	379.93	379.93
Mass Flow	lb/h	159,596.51	159,596.51
Vapor Volumetric Flow	ft ³ /h	2,843.23	3,581.73
Liquid Volumetric Flow	gpm	354.48	446.55
Std Vapor Volumetric Flow	MMSCFD	3.46	3.46
Std Liquid Volumetric Flow	sgpm	311.14	311.14
Species flow rate	lb/h		
Bottoms		159,596.51	159,596.51

Table A-6 Continued

Stream		5	6	7	8
Temperature	°F	791.59	636.17	122	122
Pressure	atm	85.86	85.73	84.37	84.37
Mole Fraction Vapor	%	95.77	88.52	100	0
Mole Fraction Light Liquid	%	4.23	11.48	0	100
Molecular Weight	lb/lbmol	37.95	37.95	2.63	140.73
Mass Density	lb/ft ³	3.57	4.21	0.5	52.79
Molar Flow	lbmol/h	4,374.75	4,374.75	3,255.79	1,118.96
Mass Flow	lb/h	166,034.9 0	166,034.9 0	8,569.42	157,465.4 8
Vapor Volumetric Flow	ft ³ /h	46,569.59	39,471.00	17,173.48	2,982.98
Liquid Volumetric Flow	gpm	5,806.08	4,921.06	2,141.11	371.9
Std Vapor Volumetric Flow	MMSCFD	39.84	39.84	29.65	10.19
Std Liquid Volumetric Flow	sgpm	553.57	553.57	186.13	367.44
Species flow rate	lb/h				
Gas Oil		76,487.16	76,487.16	0.01	76487.15
Hydrogen		6,438.39	6,438.39	6367.79	70.6
NH ₃		2,872.74	2,872.74	1311.53	1561.21
Hydrogen Sulfide		1,101.22	1,101.22	583.37	517.85
Naphtha		66,673.13	66,673.13	306.73	66366.39
Bottoms		12,462.27	12,462.27	0	12462.27

Table A-6 Continued

Stream		9	10	Purge
Temperature	°F	32	32	32
Pressure	atm	83	83	83
Mole Fraction Vapor	%	0	100	100
Mole Fraction Light Liquid	%	100	0	0
Molecular Weight	lb/lbmol	79.13	2.54	2.54
Mass Density	lb/ft ³	50.83	0.56	0.56
Molar Flow	lbmol/h	3.74	3,252.05	97.56
Mass Flow	lb/h	295.99	8,273.44	248.2
Vapor Volumetric Flow	ft ³ /h	5.82	14,800.69	444.02
Liquid Volumetric Flow	gpm	0.73	1,845.28	55.36
Std Vapor Volumetric Flow	MMSCFD	0.03	29.62	0.89
Std Liquid Volumetric Flow	sgpm	0.78	185.35	5.56
Species flow rate	lb/h			
Gas Oil		0.00750576	9.05E-10	2.71E-11
Hydrogen		0.15274405	6367.6373	191.02912
NH3		16.645884	1294.8815	38.846444
Hydrogen Sulfide		4.51750642	578.84868	17.36546
Naphtha		274.665408	32.067952	0.9620386
Bottoms		9.26E-10	3.37E-24	1.01E-25

Table A-6 Continued

Stream		11	H2 Makeup	12
Temperature	°F	32	100	52.02
Pressure	atm	83	13.61	13.61
Mole Fraction Vapor	%	100	100	100
Mole Fraction Light Liquid	%	0	0	0
Molecular Weight	lb/lbmol	2.54	2.02	2.41
Mass Density	lb/ft ³	0.56	0.07	0.09
Molar Flow	lbmol/h	3,154.49	1,126.02	4,280.51
Mass Flow	lb/h	8,025.23	2,269.92	10,295.15
Vapor Volumetric Flow	ft ³ /h	14,356.67	34,090.25	118,495.64
Liquid Volumetric Flow	gpm	1,789.92	4,250.21	14,773.48
Std Vapor Volumetric Flow	MMSCFD	28.73	10.26	38.99
Std Liquid Volumetric Flow	sgpm	179.79	64.04	243.83
Species flow rate	lb/h			
Gas Oil		8.78E-10	0	8.78E-10
Hydrogen		6176.6	2,269.92	8446.52
NH3		1256.03	0	1256.03
Hydrogen Sulfide		561.48	0	561.48
Naphtha		31.1	0	31.1
Bottoms		3.27E-24	0	3.27E-24

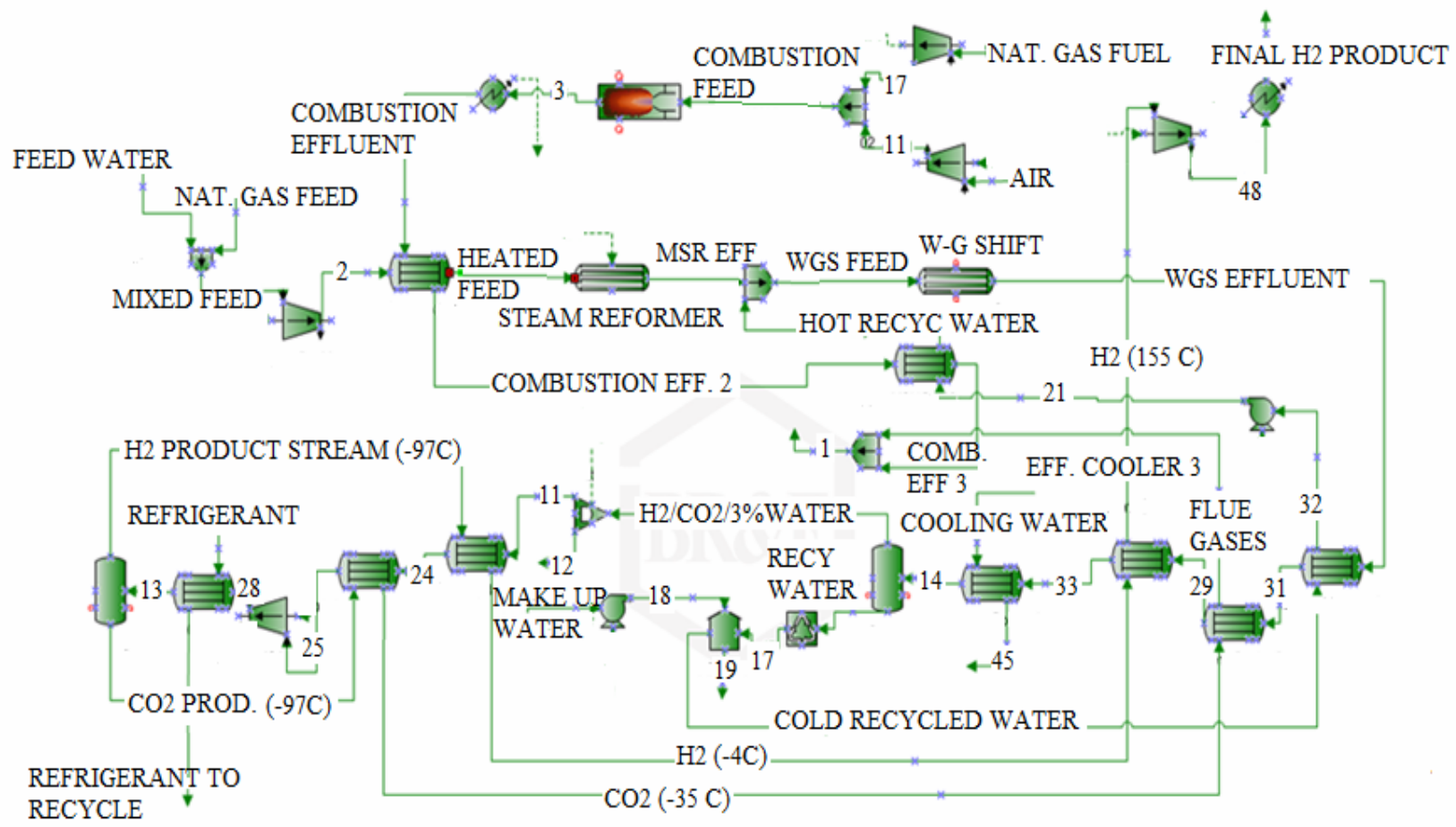


Figure A-7 Air-fired Hydrogen Plant Schematic

Table A-7 Air-fired Hydrogen Plant Composition

		Feed Water	Nat. Gas Feed	Mixed Feed	2
Temperature	°F	68	68	54.72	95.96
Pressure	atm	1.02	1.02	1.02	41.51
Mole Fraction Vapor	%	0	100	51.61	50.77
Mole Fraction Light Liquid	%	100	0	48.39	49.23
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	18.02	16.04	17.02	17.02
Mass Density	lb/ft ³	62.29	0.35	0.74	24.18
Molar Flow	lbmol/h	429.9	440.92	870.83	870.83
Mass Flow	lb/h	7,744.79	7,073.51	14,818.31	14,818.31
Vapor Volumetric Flow	ft ³ /h	124.33	19,982.83	19,971.05	612.86
Liquid Volumetric Flow	gpm	15.5	2,491.37	2,489.90	76.41
Std Vapor Volumetric Flow	MMSCFD	3.92	4.02	7.93	7.93
Std Liquid Volumetric Flow	sgpm	15.48	47.16	62.64	62.64
Species flow rate	lb/h				
Methane		0	7,073.51	7,073.51	7,073.51
Toluene		0	0	0	0
Carbon Dioxide		0	0	0	0
Carbon Monoxide		0	0	0	0
Water		7,744.79	0	7,744.79	7,073.51
Hydrogen		0	0	0	0
Ammonia		0	0	0	0

Table A-7 Continued

		Heated Feed	MSR Eff.	WGS Feed	WGS Effluent
Temperature	°F	1,634.00	5,813.25	590	640.87
Pressure	atm	40.83	40.15	40.15	39.47
Mole Fraction Vapor	%	100	100	100	100
Mole Fraction Light Liquid	%	0	0	0	0
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	17.02	8.56	17.09	17.09
Mass Density	lb/ft ³	3.76	0.62	7.97	7.34
Molar Flow	lbmol/h	870.83	1,730.63	17,162.99	17,162.99
Mass Flow	lb/h	14,818.31	14,818.31	293,291.23	293,291.23
Vapor Volumetric Flow	ft ³ /h	3,945.75	23,814.30	36,800.63	39,955.63
Liquid Volumetric Flow	gpm	491.94	2,969.06	4,588.13	4,981.48
Std Vapor Volumetric Flow	MMSCFD	7.93	15.76	156.31	156.31
Std Liquid Volumetric Flow	sgpm	62.64	104.89	661.81	686.27
Species flow rate	lb/h				
Methane		7,073.51	176.84	176.85	176.85
Toluene		0	0	537.08	537.08
Carbon Dioxide		0	12,041.58	42.36	18,851.49
Carbon Monoxide		0	0	12,041.58	70.4
Water		14,818.31	0	277,851.79	270,152.27
Hydrogen		0	2,599.89	2,599.89	3,461.45
Ammonia		0	0	41.7	41.7

Table A-7 Continued

		29	33	14	31
Temperature	°F	381.44	379.71	176	383.11
Pressure	atm	38.11	37.43	36.74	38.79
Mole Fraction Vapor	%	90.25	89.07	12.97	91.24
Mole Fraction Light Liquid	%	9.75	10.93	87.03	8.76
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	17.09	17.09	17.09	17.09
Mass Density	lb/ft ³	10.96	10.87	37.4	11.06
Molar Flow	lbmol/h	17,162.99	17,162.9	17,162.99	17,162.99
Mass Flow	lb/h	293,291.2	293,291	293,291.2	293,291.23
Vapor Volumetric Flow	ft ³ /h	26,765.58	26,982.4	7,841.30	26,510.78
Liquid Volumetric Flow	gpm	3,337.01	3,364.04	977.62	3,305.24
Std Vapor Volumetric Flow	MMSCFD	156.31	156.31	156.31	156.31
Std Liquid Volumetric Flow	sgpm	686.27	686.27	686.27	686.27
Species flow rate	lb/h				
Methane		176.85	176.85	176.85	176.85
Toluene		537.08	537.08	537.08	537.08
Carbon Dioxide		18,851.49	18,851.4	18,851.49	18,851.49
Carbon Monoxide		70.4	70.4	70.4	70.4
Water		270,152.2	270,152.	270,152.2	270,152.27
Hydrogen		3,461.45	3,461.45	3,461.45	3,461.45
Ammonia		41.7	41.7	41.7	41.7

Table A-7 Continued

		H ₂ /CO ₂ / 3 Water	12	11	24
Temperature	°F	175.99	175.99	175.99	46.4
Pressure	atm	36.68	36.68	36.68	36
Mole Fraction Vapor	%	100	0	100	100
Mole Fraction Light Liquid	%	0	100	0	0
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	10.66	18.02	10.44	10.44
Mass Density	lb/ft ³	6.97	60.7	6.81	8.44
Molar Flow	lbmol/h	2,225.37	67.12	2,158.24	2,158.24
Mass Flow	lb/h	23,732.81	1,209.22	22,523.59	22,523.5
Vapor Volumetric Flow	ft ³ /h	3,407.27	19.92	3,308.66	2,668.09
Liquid Volumetric Flow	gpm	424.8	2.48	412.51	332.65
Std Vapor Volumetric Flow	MMSCFD	20.27	0.61	19.66	19.66
Std Liquid Volumetric Flow	sgpm	147.18	2.42	144.76	144.76
Species flow rate	lb/h				
Methane		176.84	0	176.84	176.84
Toluene		2.29	0	2.29	2.29
Carbon Dioxide		18,809.18	0	18,809.1	18,809.1
Carbon Monoxide		70.4	0	70.4	70.4
Water		1,209.22	1,209.2	0	0
Hydrogen		3,461.45	0	3,461.45	3,461.45
Ammonia		3.43	0	3.43	3.43

Table A-7 Continued

		25	28	13	CO ₂ Product Stream (- 97 C)
Temperature	°F	-4	-0.91	-142.6	-142.63
Pressure	atm	35.32	38.72	559	37.97
Mole Fraction Vapor	%	100	100	86.26	0
Mole Fraction Light Liquid	%	0	0	13.74	100
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	10.44	10.44	10.44	43.98
Mass Density	lb/ft ³	9.24	10.06	14.78	81.63
Molar Flow	lbmol/h	2,158.24	2,158.24	2,158.24	296.4
Mass Flow	lb/h	22,523.59	22,523.59	22,523.59	13,036.78
Vapor Volumetric Flow	ft ³ /h	2,437.17	2,238.96	1,524.10	159.71
Liquid Volumetric Flow	gpm	303.85	279.14	190.02	19.91
Std Vapor Volumetric Flow	MMSCFD	19.66	19.66	19.66	2.7
Std Liquid Volumetric Flow	sgpm	144.76	144.76	144.76	31.71
Species flow rate	lb/h				
Methane		176.84	176.84	176.84	1.11
Toluene		2.29	2.29	2.29	2.29
Carbon Dioxide		18,809.18	18,809.18	18,809.18	13,029.86
Carbon Monoxide		70.4	70.4	70.4	0.05
Water		0	0	0	0
Hydrogen		3,461.45	3,461.45	3,461.45	0.08
Ammonia		3.43	3.43	3.43	3.39

Table A-7 Continued

		Flue gases	1	Combustion Eff 3	Combustion Eff 2
Temperature	°F	320	60.29	58.28	193.42
Pressure	atm	36.61	1.02	1.02	1.7
Mole Fraction Vapor	%	100	84.58	83.76	100
Mole Fraction Light Liquid	%	0	15.42	16.24	0
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	43.98	28.34	27.76	27.76
Mass Density	lb/ft ³	24.66	0.75	0.74	0.82
Molar Flow	lbmol/h	296.4	8,299.18	8,002.78	8,002.78
Mass Flow	lb/h	13,036.7	235,179	222,143.15	222,143.15
Vapor Volumetric Flow	ft ³ /h	528.75	314,125	298,873.20	269,501.91
Liquid Volumetric Flow	gpm	65.92	39,163.6	37,262.11	33,600.24
Std Vapor Volumetric Flow	MMSCFD	2.7	75.59	72.89	72.89
Std Liquid Volumetric Flow	sgpm	31.71	565.05	533.34	533.34
Species flow rate	lb/h				
Methane		1.11	1.33	0.23	0.23
Toluene		2.29	2.29	0	0
Carbon Dioxide		13,029.8	45,047.2	32,017.41	32,017.41
Carbon Monoxide		0.05	0.05	0	0
Water		0	26,212.6	26,212.64	26,212.64
Hydrogen		0.08	0.08	0	0
Ammonia		3.39	3.39	0	0
Nitrogen		0	161,005.	161,005.65	161,005.65
Oxygen			0.91	0.91	0.91
Argon			2,906.32	2,906.32	2,906.32

Table A-7 Continued

		CO ₂ (-35 C)	Combustion Eff	3
Temperature	°F	-36.27	650	4,790.54
Pressure	atm	37.29	2.38	2.72
Mole Fraction Vapor	%	0	100	100
Mole Fraction Light Liquid	%	100	0	0
Mole Fraction Heavy Liquid	%	0	0	0
Molecular Weight	lb/lbmol	43.98	27.76	27.76
Mass Density	lb/ft ³	69.44	0.68	0.16
Molar Flow	lbmol/h	296.4	8,002.78	8,002.78
Mass Flow	lb/h	13,036.78	222,143.15	222,143.15
Vapor Volumetric Flow	ft ³ /h	187.74	327,628.32	1,356,329.49
Liquid Volumetric Flow	gpm	23.41	40,847.17	169,100.82
Std Vapor Volumetric Flow	MMSCFD	2.7	72.89	72.89
Std Liquid Volumetric Flow	sgpm	31.71	533.34	533.34
Species flow rate	lb/h			
Methane		1.11	0.23	0.23
Toluene		2.29	0	0
Carbon Dioxide		13,029.86	32,017.41	32,017.41
Carbon Monoxide		0.05	0	0
Water		0	26,212.64	26,212.64
Hydrogen		0.08	0	0
Ammonia		3.39	0	0
Nitrogen		0	161,005.65	161,005.65
Oxygen		0	0.91	0.91
Argon		0	2,906.32	2,906.32

Table A-7 Continued

		Combustion Feed	47	41	Nat. Gas. Fuel
Temperature	°F	719.3	639.8	735.25	674
Pressure	atm	2.72	2.76	2.72	14.63
Mole Fraction Vapor	%	100	100	100	100
Mole Fraction Light Liquid	%	0	0	0	0
Mole Fraction Heavy Liquid	%	0	0	0	0
Molecular Weight	lb/lbmol	27.76	16.04	28.93	16.04
Mass Density	lb/ft ³	0.73	0.45	0.75	0.45
Molar Flow	lbmol/h	8,002.78	727.53	7,275.25	727.53
Mass Flow	lb/h	222,143.15	11,671.3	210,471.8	11,671.3
Vapor Volumetric Flow	ft ³ /h	304,736.50	25,821.2	280,788.3	4,964.19
Liquid Volumetric Flow	gpm	37,993.12	3,219.28	35,007.37	618.91
Std Vapor Volumetric Flow	MMSCFD	72.89	6.63	66.26	6.63
Std Liquid Volumetric Flow	sgpm	562.36	77.81	484.56	77.81
Species flow rate	lb/h				
Methane		11,671.30	11,671.3	0	11,671.3
Hydrogen		0	0	0	0
Nitrogen		161,005.65	0	161,005.6	0
Oxygen		46,559.88	0	46,559.88	0
Argon		2,906.32	0	2,906.32	0

Table A-7 Continued

		Air	Hydro Prod. Stream -97	H2 (-4 C)
Temperature	°F	674	-142.63	25.15
Pressure	atm	1.02	37.97	37.29
Mole Fraction Vapor	%	100	100	100
Molecular Weight	lb/lbmol	28.93	5.1	5.1
Mass Density	lb/ft ³	0.3	6.94	4.41
Molar Flow	lbmol/h	7,275.25	1,861.84	1,861.84
Mass Flow	lb/h	210,471.85	9,486.81	9,486.81
Vapor Volumetric Flow	ft ³ /h	709,955.47	1,366.68	2,151.18
Liquid Volumetric Flow	gpm	88,513.93	170.39	268.2
Std Vapor Volumetric Flow	MMSCFD	66.26	16.96	16.96
Std Liquid Volumetric Flow	sgpm	484.56	113.05	113.05
Species flow rate	lb/h			
Hydrogen		0	9,486.81	9,486.81
Nitrogen		161,005.65	0	0
Oxygen		46,559.88	0	0
Argon		2,906.32	0	0

Table A-7 Continued

		48	Final H2 Product
Temperature	°F	374	752
Pressure	atm	136.43	136.43
Mole Fraction Vapor	%	100	100
Molecular Weight	lb/lbmol	5.1	5.1
Mass Density	lb/ft ³	9.04	9.04
Molar Flow	lbmol/h	1,861.84	1,861.84
Mass Flow	lb/h	9,486.81	9,486.81
Vapor Volumetric Flow	ft ³ /h	1,048.93	1,048.93
Liquid Volumetric Flow	gpm	130.78	130.78
Std Vapor Volumetric Flow	MMSCFD	16.96	16.96
Std Liquid Volumetric Flow	sgpm	113.05	113.05
Species flow rate	lb/h		
Hydrogen		9,486.81	9,486.81

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