

ECONOMICS OF STEAM METHANE REFORMATION AND COAL GASIFICATION FOR  
HYDROGEN PRODUCTION

By

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To my family for their continuous love, support, and encouragement.

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Fossil fuels (especially petroleum) drive today's leading economies. However, soon that age will decline, and we will need alternatives less detrimental to our environment. Hydrogen continues to be one of the most promising, talked about energy carriers of the future. Cost-effective, more environmental friendly methods of producing hydrogen need to be commercially established. In addition storage and transportation continue to remain dominant hurdles that need to be improved. We performed an economic comparison of two methods for producing hydrogen commercially – steam methane reformation and coal gasification; to reach a solution that will most benefit future generations.



## CHAPTER 1 BACKGROUND INFORMATION

### 1.1 Introduction

The world is approaching the first stages of an energy crisis that could have a serious impact on the security, economics, politics, and lifestyle of every human being. This crisis is being caused primarily because the world's economy has been dependent on oil for so long and we will soon reach a stage when the growth in demand for oil exceeds our ability to supply it and we do not have commercially viable alternatives. There are no immediate solutions to this problem but the repercussions in the near future will be severe, which is why we need to act soon.

We have faced similar situations before (most notably the oil crises in 1973, 1979 and more recently in 1990, 2001 and 2003 onwards) that arose due to political reasons. In the United States, the price of oil rose from \$3/bbl to almost \$40/bbl in the 1970s alone. For the handful of industrialized nations like the Soviet Union that were net energy exporters the effects of the oil crisis resulted in a sudden and massive influx of money. Experts attribute the recent spike to \$78/bbl in 2006 to a variety of factors: North Korea's missile launches, the crisis between Israel and Lebanon, Iranian nuclear brinkmanship, and most importantly because of reports from the U.S Department of Energy confirming a decline in petroleum reserves.

Evidence of this is the fact that oil companies spent \$8 billion on exploration in 2003, but discovered only \$4 billion of commercially useful oil [1]. More proof is Chevron Texaco's recent decision to acquire an oil company and its reserves last year which reveals that bigger oil companies consider it cheaper to just buy oil than invest in exploration [2].

In recent years, even oil producing nations have been unable to keep pace with fast growing global demand. The fact that oil has increased from below \$25/bbl since 2003 to

\$63/bbl today, while oil producers have consistently produced at maximum capacity, is compelling evidence that oil is becoming scarce relative to demand and that there are no more oil reserves available.

Peak oil is the inevitable movement when world oil production hits its peak and, from that moment on, reserves are on an ever dwindling downward spiral. By the end of 2005, British Petroleum estimated the world oil reserves at 1.2 trillion barrels and at our current consumption rate of about 83 million barrels per day; we barely have enough to last another 40 years. According to the U.S. Energy Information Agency, the United States is the single largest consumer of oil worldwide at about 25% followed by China and Japan at 8% and 6% each.

A policy of conservation of energy should be enforced. Conservation measures and steps to improve existing efficiencies can lower the rate of increased demand imposed by worldwide economic development and increase in population. And while it may be a step in the right direction there is no single solution to avoid the long period of energy shortages we will soon enter. By acknowledging that these shortages are real and permanent, there are many things we can do both individually and as a global economy to make the most from the world energy crisis which has already begun. It is the steady rise in oil prices that will force alternative energy sources that are already environmentally sound and commercially attractive for future use even though they may appear more capital intensive. We need to act now to develop the infrastructure this transition requires since there is none to provide fuels in the volumes required if we hope to one day replace our current use of oil. Installing this kind of infrastructure will take years.

Finally the greenhouse effect and pollution are just a few of the environmental problems caused by the utilization of fossil fuels. One of the main pollutants is carbon dioxide. The U.S. Energy Information Agency reports that carbon dioxide accounts for about 83% of the

greenhouse gases released into the atmosphere. The continuing carbon dioxide pollution to the environment is causing global warming (in turn, affecting forests, agriculture yields, ecosystems, as well as human health and well-being). The information provided in this section should prove without any doubt that the world energy crisis is very real and we need to adopt alternative sources of energy that are less polluting.

## **1.2 Why Hydrogen?**

One fuel that is expected to play a major role in the mid to long-term future of the energy sector is hydrogen. Hydrogen is a desirable fuel for various reasons as discussed below.

Hydrogen, the lightest element, has three isotopes: hydrogen, H, deuterium, D and tritium, T [3]. Hydrogen is abundant and available in plenty as water occupying about 70% of the earth's surface.

Whereas hydrogen atoms exist under certain conditions, the normal state of pure hydrogen is the hydrogen molecule,  $H_2$ , which is the lightest of all gases. Molecular hydrogen is a product of many reactions, but is present at only low levels (0.1 ppm) in the Earth's atmosphere. The hydrogen molecule exists in two forms, designated ortho-hydrogen and para-hydrogen, depending on the nuclear spins of the atoms. Many physical and thermodynamic properties of  $H_2$  depend on the nuclear spin orientation, but the chemical properties of the two forms are the same.

Compared to other possible alternatives hydrogen has the highest energy content per unit weight of 120 MJ/kg as opposed to 48 MJ/kg for natural gas and 44 MJ/kg for gasoline [4]. It is a very stable molecule and is not particularly reactive under normal conditions. However, at elevated temperatures and with the aid of catalysts,  $H_2$  undergoes many reactions and forms compounds with almost every other element.

Hydrogen energy has long been established scientifically as an environmentally cleaner source of energy to end-users, particularly in transportation applications without significant release of pollutants. Upon combustion, hydrogen returns to water, accompanied by virtually no pollution and no greenhouse gas production, in contrast to hydrocarbon-based fuels. Since U.S. transportation is 97% dependent on petroleum, (much of it imported from parts of the world that are considered politically unstable), a strategy of shifting to domestically-produced hydrogen fuel is very appealing.

However, there are several key issues that need to be addressed. Safety, storage and transportation of hydrogen continue to remain major areas that need further improvement if we are to support the large capital investments needed to develop the vast infrastructure that will propel hydrogen as the energy source of the future. However significant scientific progress has been made in these fields over the last decade that has generated growing interest worldwide.

Hydrogen is a product that is fully capable of sustaining the world's energy needs now and in the future. If renewably produced, hydrogen would be a fuel used that does not contribute to environmental damage and supports the human well being.

### **1.3 The Hydrogen Economy**

In virtually all advanced economies, there is considerable interest and enthusiasm over the concept of a hydrogen economy and the prospect of hydrogen-fuelled vehicles. Not since the mid 1970s, when the term “hydrogen economy” was first coined, has there been anything like the current level of research activity and discussion even in the popular press.

Several examples of large-scale hydrogen based energy systems can be cited. Among them are the World Energy Network (WE-NET) in Japan [5], the Solar Hydrogen Demonstration Plant in Neunburg vorm Wald [6] and the HYSOLAR: A German-Saudi Arabian Program on Solar Hydrogen [7]. The best example that can be cited is the FutureGen Alliance, a non-profit

consortium of some of the world's largest coal producers and users formed to partner with the U.S. Department of Energy's FutureGen project. Member companies span Australia, Canada and China. These projects are aimed at establishing a worldwide energy system based on harnessing sources such as solar and coal, producing hydrogen via water electrolysis, and liquefying the hydrogen to the end points of use. Current efforts are to design efficient water electrolyzers, large-scale hydrogen liquefaction plants and high efficiency hydrogen gas turbines.

There are still many technical hurdles yet to be fully overcome involved with the safe transportation and storage of hydrogen. The challenge may be summarized thus: manufacturers are unwilling to produce vehicles without an in-place fuelling infrastructure and fuel producers are unwilling to build that infrastructure without some certainty that vehicles requiring those fuels will be in operation.

From a transportation perspective, generally what is envisioned is fuel cell powered cars that use hydrogen as fuel and produce only water vapor as emissions. A fuel cell is an energy conversion device that combines hydrogen and oxygen in an electrochemical process to produce electric power, some low temperature heat and water vapor as the only emissions. The use of liquid hydrogen as a rocket fuel for use in space flights is well established and is now being seriously considered for use as fuel for aircraft.

Unfortunately, 96% of all hydrogen produced in the U.S. today uses natural gas as a feedstock in spite of having the world's largest reserves of coal. The trends in natural gas prices follow trends in the price of oil. Therefore the cost of producing hydrogen becomes dependent on the highly volatile price of natural gas.

For most rapidly developing and developed nations, the best alternative to natural gas is coal which is cheaper and more readily available. Today coal is priced as a dirty solid fuel and

for this reason it is often available at a small fraction of the cost of cleaner oil and natural gas containing the same amount of energy. The process of commercial production of hydrogen along with electricity, industrial grade process steam and pre-cursors to produce usable transportation fuels from coal, coke and other carbonaceous matter is called IGCC or Integrated Gasification Combined Cycle.

For more than 40 years the South African government, fearing an oil embargo in retaliation to their policy of apartheid, has commercially produced a range of liquid fuels from coal including gasoline, diesel and jet fuel.

Countries such as the U.S., China and India that are oil-poor but coal rich could stand to benefit greatly and could potentially convert its principal asset for energy independence! Today, no single technology seems to offer a clear solution, although it appears that coal gasification offers a potential solution with respect to sustainability issues and energy independence, many technical hurdles remain which suggest it is decades away from large scale, cost effective implementation.

Given these many uncertainties, one might argue that it is premature to analyze alternative forms of infrastructure. However, if one accepts the premise of a not-so distant hydrogen transition and the need to begin making the necessary investments now, strategic planning need not wait for resolution of these many issues. Rather, energy, economic and environmental analyses must be undertaken in concert with research on improved production, storage, and distribution technologies.

Table 1-1. Properties of Selected Fuels

| Property  | Hydrogen<br>H <sub>2</sub> | Methane<br>CH <sub>4</sub> | Methanol<br>CH <sub>3</sub> OH | Gasoline<br>C <sub>6</sub> -C <sub>12</sub> |
|---|----------------------------|----------------------------|--------------------------------|---|
| Boiling point, °C                                   | -253                       | -162                       | 65                             | Wide range                                  |
| Physical state at 25°C                              | Gas                        | Gas                        | Liquid                         | Liquid                                      |
| Heating value: weight basis                         |                            |                            |                                |   |
| Lower heating value, MJ/kg                          | 120                        | 48                         | 20                             | 42-44                                       |
| Higher heating value, MJ/kg                         | 142                        | 53                         | 23                             | 44-46                                       |
| Heating value: volume basis*                        |                            |                            |                                |   |
| Lower heating value, MJ/Nm <sup>3</sup>             | 11                         | 35                         | 15,700                         | -32,000                                     |
| Higher heating value, MJ/Nm <sup>3</sup>            | 13                         | 39                         | 18,100                         | -33,000                                     |
| Flammability limits, vol. % in air                  | 4.1 to 74.0                | 5.3 to 15.0                | 6.0 to 36.5                    | 1.4 to 7.6                                  |
| Explosive limits, vol. % in air                     | 18.2 to 58.9               | 5.7 to 14.0                | 6.7 to 36.0                    | 1.4 to 3.0                                  |
| Molecular diffusion coefficient, cm <sup>2</sup> /s | 0.61                       | 0.16                       | 0.13                           | 0.05  |
| Auto-ignition temperature in air, °C                | 571                        | 632                        | 470                            | 220   |

\* Nm<sup>3</sup> of gas at atmospheric pressure or m<sup>3</sup> of liquid

## CHAPTER 2 HYDROGEN PRODUCTION METHODS

There are several methods of producing hydrogen today. Those that will be discussed and compared in this study are steam methane reformation (SMR) and gasification. A brief discussion of both technologies will be made followed by an economical analysis in the subsequent chapters in an attempt to reach a solution that will prove most advantageous for near-term effect and promote energy independence.

Hydrogen production methods from renewable sources have not been considered in this analysis for several reasons. They tend to be an intermittent source of energy that is not yet completely reliable without the use of advanced storage methods. Consequently this results in huge initial investments and cannot be deemed a practical solution when compared to more commercially methods already in existence today. The initial hurdle lies in establishing these existing technologies on a larger global scale following which enough industrial experience of related supporting technologies can be better understood to equip us for future implementation of production methods from renewable sources.

Today, hydrogen is produced primarily from fossil fuels (natural gas, petroleum, and coal) using well-known commercial processes. Worldwide, the predominant feed is natural gas (48%), followed by oil–petroleum (30%), coal (18%), and electricity (4%) [8]. The process description that follows is not meant to provide a detailed understanding but a brief overview comparing both technologies that lead to the process economics.

### **2.1 Steam Methane Reformation (SMR)**

#### **2.1.1 Introduction**

Large-scale catalytic steam reformation of natural gas is the most common, least expensive method of producing hydrogen commercially available today and almost 48% of the world's



hydrogen is produced from SMR. Natural gas is, on average, ~ 95% methane, with the balance being higher hydrocarbons (ethane, propane) and trace contaminants, such as H<sub>2</sub>S and CO<sub>2</sub>. SMR is widely used, especially in the United States, to provide high purity hydrogen to the chemical, petrochemical, and refining industries.

### 2.1.2 Process Description

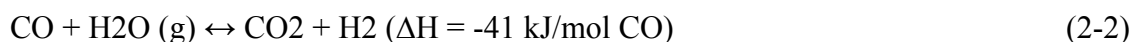
This method is a multi-step process that comprises of gas pre-treatment; catalytic reforming; high temperature water–gas shift; low temperature water–gas shift; purification; and compression/liquefaction. Descriptions of each major component technology are based on Figure 2-1.

- **Feedstock:** Natural gas to be used must be compressed before it undergoes reformation. Feed pre-treatment is generally required, since untreated natural gas nearly always contains sulfur compounds. Pre-treatment and handling of compressed natural gas is easier and cheaper than that required for coal or any other solid carbonaceous matter used in gasification.
- **Purification (Desulfurization):** After the feed is compressed, natural gas undergoes desulfurization to remove traces of sulfur from the gas. Desulfurization of the feed gas, which is usually carried out using a zinc oxide bed, is needed since sulfur can poison the reformer catalyst.
- **Selective Catalytic Reduction (SCR):** Low NO<sub>x</sub> burner technology is sometimes not able to meet strict regulations alone and therefore, new SMRs also require the addition of an SCR unit to the stack. Here liquid ammonia is vaporized and injected into the flue gas, which passes over a honeycomb-shaped (V<sub>2</sub>O<sub>5</sub> – TiO<sub>2</sub>) catalyst. The ammonia reacts with NO<sub>x</sub> in the presence of oxygen to form nitrogen and water vapor. By varying the ammonia injection rate, NO<sub>x</sub> is controlled to the desired level.
- **Reformation:** After pre-treatment, the feed gas is mixed with process steam at an appropriate steam-to-carbon mole ratio of 3 (typically) to prevent the production of solid carbon or coke, which can build up on the catalyst and plug the reactor tubes. The catalytic steam reforming reaction takes place at pressures of approximately 3-25 bar and high temperatures (650-900°C) [8]. The reformation is favored by high temperature and steam and reduced by higher pressure. Recent advancements (e.g., high pressure catalyst tubes) in reformer technology allow reliable hydrogen production even at higher operating pressures.



The catalyst, typically nickel based, is packed into tubes and the heat needed for reaction shown above is provided externally by combustion of additional natural or purge gas. Concerns regarding emissions can be addressed by using the latest environmental controls for NO<sub>x</sub> control and sulfur removal while designing an SMR facility. Environmental controls significantly add to the capital and operating costs of a hydrogen production facility. The SMR process is a more environmentally acceptable process of producing hydrogen than gasification. Low NO<sub>x</sub> burners utilize staged fuel combustion and flue gas recirculation to minimize NO<sub>x</sub> production. (Staged fuel combustion involves introducing the fuels at different locations to create two combustion zones). Tail gas from the Pressure Swing Adsorption (PSA) unit provides bulk of the heat input to the furnace, with natural gas for start up and control. Once the reformer is heated, the unit can operate with 100% PSA fuel if needed. The basic layout has the convection section and the stack mount on top, with a process gas waste heat boiler located underneath. A steam drum is mounted on top of the reformer.

- **Shift:** The synthesis gas mixture (“syngas” is a mixture of hydrogen and CO) is sent to the high and low temperature shift reactors, where additional hydrogen is produced via the water–gas shift reaction:



The above reaction is favored at lower temperatures as opposed to the reformer reaction. To compensate for slower reaction kinetics at lower temperatures a solid Co-Mo catalyst is used. To take advantage of the high temperatures generated, a two-stage water-gas shift reaction is generally used, with the high temperature stage operating at ~ 400°C and the low temperature stage at ~ 250°C. The exit gas contains primarily H<sub>2</sub>, and also CO<sub>2</sub>, H<sub>2</sub>O and small amounts of CO, methane and higher hydrocarbons. Since residual CO leaving the shift converter is recovered in the PSA unit as reformer fuel, the gain in plant efficiency if a second stage of shift is added is less when compared to the increase in equipment cost. The costs involved for the shift reactions are high, but lower when compared to the same process taking place in gasification. This can be attributed to the higher amounts of steam required to shift the larger amounts of CO generated for an equivalent amount of hydrogen.

- **Pressure swing adsorption (PSA):** After cooling of the raw gas and separation of process condensate, a PSA unit is used to purify the raw H<sub>2</sub>. They operate at about 20 bar and reach H<sub>2</sub> separation efficiencies in the range 85–90%. It is the most common process used in large systems, where very high purity hydrogen (99.999%) at ~ 30 bar is the desired product. These PSA-based hydrogen plants have higher efficiencies than conventional low-purity plants because of additional export steam credits. The adsorbent used is a mixture of activated carbon and zeolites and removes all of the contaminants from the hydrogen product in a single step. With adjustments to the PSA operation, one can also produce a high purity CO<sub>2</sub> stream for sequestration or for sale, in addition to the hydrogen stream but at the cost of hydrogen purity [9]. Tail gas from the PSA unit is used as reformer fuel. Again the costs involved with the PSA units are high but lower than a similar arrangement in gasification which will be described further on.

- **Compression:** Following the PSA purification step, hydrogen gas is compressed to ~ 60 bar and sent to steam generators as shown in the Figure 2-1.
- **Heat recovery:** Heat recovery coils include feed gas preheat, mixed feed (gas and steam) preheat, steam generation, and steam superheating. The reformer furnace process outlet is cooled in a waste heat boiler by heat exchange with circulating feed-water to produce steam. This steam can be exported to a nearby refinery or petrochemical facility for process needs and/or converted into electricity. Downstream of the shift converter, the gas is cooled against boiler feed-water.

## 2.2 Gasification

### 2.2.1 Introduction

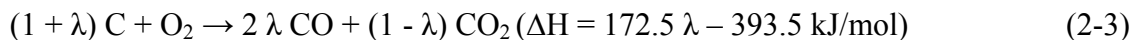
Coal has been used for centuries with the earliest recorded use in China in 220 A.D. Later on in the 1600s when coal was heated and the release of gas was first noted, the process was described as “the coal did belch forth a wild spirit or breath . . . not susceptible of being confined in vessels, nor capable of being reduced to a visible body.”

Coal gasification is the process of reacting coal with oxygen, steam, and carbon dioxide to form a product gas containing hydrogen and carbon monoxide. Gasification is essentially incomplete combustion. From a processing point of view the main operating difference is that gasification consumes heat evolved during combustion. Depending on the type of gasifier and the operating conditions, gasification can be used to produce a fuel gas suitable for any number of applications. For instance, a low heating value fuel gas may be produced from an air blown gasifier for use as an industrial fuel and for power production. A medium heating value fuel gas may be produced from enriched oxygen blown gasification for use as a synthesis gas in the production of chemicals such as ammonia, methanol, and transportation fuels. A high heating value gas can be produced from shifting the medium heating value product gas over catalysts to produce a substitute or synthetic natural gas (SNG). The technical information described here is very similar to commercially available systems in IGCCs.

### 2.2.2 Process Description

The flexibility of gasification technology allows it to be integrated into a variety of system configurations to produce electrical power, thermal energy, fuels, or chemicals as shown in Figure 2-2. This section provides a brief description of each major component technology.

- **Raw materials:** The raw material used in the gasifier is fed as slurry. Gasifier feed (coal), is ground in mills and treated with pre-heated water to the required mixture. As indicated in the diagram, a vast array of carbonaceous matter can be used as feedstock for gasification. The advantages of flexible feedstock are outweighed however by the fact that storage, pre-treatment and handling is much more cumbersome and thus capital-intensive than using natural gas for SMR. This is one of several factors that make gasification more expensive than SMR, the others associated with the air separator, removal of ash and other particulate matter, sulfur, CO<sub>2</sub> removal and sequestration, additional steam requirements for the shift reaction as compared to SMR, and finally the larger PSA system requirements which are discussed below.
- **Air separator:** The air separator is essentially a unit that generates ~ 95% pure O<sub>2</sub> at atmospheric pressure along with trace amounts of N<sub>2</sub> and Ar. The O<sub>2</sub> is then compressed to slightly higher than the gasifier operating pressure and fed to the gasifier. The purge N<sub>2</sub> is also compressed and fed to the combustion gas turbine for NO<sub>x</sub> control. The air separator is one of the components that make gasification more expensive owing to its additional power requirements and costs associated with O<sub>2</sub> compression.
- **Gasifier:** Current gasification technology takes place in O<sub>2</sub>-blown, entrained flow gasifiers operating at 70 bar. Entrained Flow Gasifiers have been developed to improve the gas production rate and can operate with a wider range of feedstock and allows complete conversion to hydrogen, carbon monoxide, and carbon dioxide, producing no tars, oils, or phenols. Coal slurry and oxygen are fed at the top of the pressurized vessel at operating temperatures of the order of 1350°C. Liquid slag flows down the walls and is drained from the lockhopper. In gasifiers partial combustion occurs in an oxygen-deficient or reducing atmosphere using about 30-50% of the oxygen theoretically required for complete combustion to carbon dioxide and water. Carbon monoxide and hydrogen are the principal products, and only a fraction of the carbon in the coal is oxidized completely to carbon dioxide. The combustion reaction is written in a general form as:



where  $\lambda$  varies from 0 (pure CO<sub>2</sub> product) to 1 (pure CO product).

The value of  $\lambda$  depends upon the gasification conditions and is usually close to 1. The heat released by the partial combustion provides the bulk of the energy necessary to drive the endothermic gasification reactions. Further conversion occurs through the much slower, reversible gasification reactions with CO<sub>2</sub> and H<sub>2</sub>O produced by gasification with heavier carbonaceous material such as waste oils.



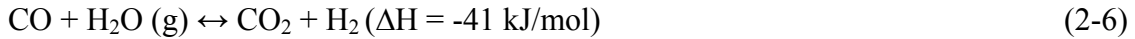
Hydrogen and carbon monoxide production increases with decreasing oxygen in the feed, with decreasing pressure, and with increasing temperature. The composition of hydrogen and carbon monoxide produced in the newer generation of gasifiers are sufficient for all applications - liquid production, chemical synthesis or power generation. As can be observed from the figure, excess steam from the heat recovery steam generator (HRSG) is drawn off and can be sold as industrial-grade process steam. The remaining steam is sent to the gasifier for further syngas production as described above and also for quench cooling to  $\sim 250^\circ\text{C}$ . Although this process results in a slight drop in efficiency, (due to the thermal energy drop in the syngas that could have been used to create valuable high pressure steam) this process is vital for two reasons – to lower the concentration of unwanted trace elements and to increase saturation that will promote the shift reactions that follow. The quenching process is quite inexpensive and reliable but nonetheless adds to the capital costs involved in this process.

- Particulate removal:** Minerals (ash) in the feedstock separate and leave the bottom of the gasifier either as an inert glass-like slag or other marketable solid product. A small fraction of the ash becomes entrained in the syngas and requires downstream particulate removal. The raw syngas after quenching is sent to a scrubber giving a saturated flow largely free of particulate matter and water-soluble contaminants such as  $\text{NH}_3$ , HCN and chlorides. Particulate removal is effected either through a series of dry solid filters, so that the gas fed to the combustion turbine is essentially free of suspended particulates. In this system first, a hot cyclone removes over 90% of the particulates, and the remainder is removed by an advanced dry char filtration system. Slag, the major solid by-product of the gasification process, is vitrified black sand like material that can be marketed as construction material. There are no solid wastes from the coal gasification process [similar to those produced by a pulverized coal process] – no scrubber sludge, fly ash or bottom ash. Gasifier slag can be used as a principal component in concrete mixtures (Slagcrete) to make roads, pads, and storage bins. Other applications of gasifier slag and fly slag are in asphalt aggregate, Portland cement kiln feed, and lightweight aggregate. In a gasification facility, heavy metals are very low because they are encapsulated in the slag. Other metals, such as mercury and selenium, are volatile and are detected in the syngas. Compared to a conventional combustion plant, metals removal should be easier because the cleanup can be done on the syngas at a higher pressure in a reducing environment rather than in the lower pressure, oxidizing environment of the effluent. Thus near-complete removal from syngas exists by selective adsorbents.
- Gas clean-up:** This stage essentially frees the syngas stream of sulfur and  $\text{CO}_2$ . Sulfur is converted to  $\text{H}_2\text{S}$  and COS under the reducing conditions of the gasifier and the COS produced is converted to  $\text{H}_2\text{S}$  at the shift reactors. The  $\text{H}_2\text{S}$  is sent to a sulfur recovery unit typically found in such processes that comprises an air-blown Claus plant for oxidizing  $\text{H}_2\text{S}$  to elemental sulfur, and a Shell Claus off-gas treating (SCOT) plant for tail gas cleanup. Claus plant tail gas contains sufficiently high levels of sulfur compounds ( $\text{H}_2\text{S}$ ,  $\text{SO}_2$ , COS,  $\text{CS}_2$  and S vapor) that require further cleanup. In the SCOT process, these

compounds are catalytically converted to  $\text{H}_2\text{S}$ , which is removed with an amine absorption unit and recycled back to the Claus plant. A Rectisol system can be used for acid gas removal from the syngas because it provides better sulfur removal than an amine system. However, a Rectisol system is more expensive and auxiliary power intensive than the amine systems. Therefore prior to  $\text{CO}_2$  capture,  $\text{H}_2\text{S}$  is removed from the syngas (containing  $\sim 0.6\%$   $\text{H}_2\text{S}$  by volume) by physical absorption in dimethyl ether of polyethylene glycol (Selexol) to elemental sulfur that can be sold at  $\sim \$100/\text{ton}$ . Sulfur removal efficiency exceeding 99% are commonly achieved in IGCCs [10, and 11]. Combustion of coal gas in high firing-temperature gas turbines converts virtually the entire  $\text{CO}$  to  $\text{CO}_2$ .  $\text{CO}_2$  removal is required since it substantially increases the heating value of the pressure swing adsorption (PSA) purge gas so as to make feasible its use in a gas turbine following compression and since it reduces the size (and thus the cost) of the PSA system.  $\text{CO}_2$  is removed from the sulfur-free syngas (containing 30-32%  $\text{CO}_2$  by volume) by physical absorption in Selexol at  $35^\circ\text{C}$ . Unlike  $\text{H}_2\text{S}$  removal, where stripping is carried out by heating the rich solvent, the  $\text{CO}_2$  is released without heating in a series of flash drums at decreasing pressures. Since  $\text{CO}_2$  emissions is a major concern with gasification a mention will be made at this point about sequestration. After  $\text{CO}_2$  is separated from the process stream, it is sequestered so it is not released to the atmosphere. The two most commonly proposed methods for sequestration are ocean disposal and underground injection [9]. In ocean disposal, several options are available - Liquid  $\text{CO}_2$  may be released from pipelines at depths of 2,000 m or more; solid  $\text{CO}_2$  can be disposed of by ships; or  $\text{CO}_2$  can be converted into hydrates for disposal. With underground sequestration, the  $\text{CO}_2$  is injected into depleted natural gas reservoirs or other geologic formations such as aquifers. Okken [9] estimates that there is a total of 5 years worth of capacity in old natural gas wells and an additional 15 years capacity in sedimentary basins. Although the ocean has a  $\text{CO}_2$  uptake capacity that is almost 7,000 times greater than current carbon emissions it cannot be considered feasible since the  $\text{CO}_2$  will not remain in the ocean for long and requires further investigation into the impacts on marine ecosystems. Ocean disposal can be considered for future implementation but not while the costs involved are approximately twice those of underground injection. Costs for removal, stripping and compression of  $\text{CO}_2$  are included from previous estimates and included in the economic analysis in the next chapter. This and the sulfur removal systems substantially increase the cost of gasification. During gasification the nitrogen content of coal is converted to molecular nitrogen,  $\text{N}_2$ , ammonia,  $\text{NH}_3$ , and a small amount of hydrogen cyanide,  $\text{HCN}$ . Other techniques are being investigated in hot-gas cleanup technologies. The lower  $\text{NO}_x$  from the combustion turbines are the result of improved turbine design and the use of a diluent (steam or  $\text{N}_2$  purge gas) for  $\text{NO}_x$  control. Since a major portion of the power generated comes from the gas turbine, the water requirement is substantially reduced from that required for a conventional coal-fired power plant, where all of the power is generated from steam turbines. The problem of water required for water-treatment systems to address tars, phenols, and metals is eliminated for entrained-flow gasifiers. The waste water from the gasification plants is cleaned up to meet the requirements for water discharges. However, if desired and at additional expense, a reverse osmosis system can be added to treat the waste water from the gasification system to obtain a zero discharge system. The water required by a gasification facility is a variable that is often neglected. Hence a rough

estimate of the water requirements of both SMR and gasification will be made to produce realistic results.

- **Shift reactor:** The mixture of H<sub>2</sub>O and CO (water-gas) shift reaction is used to “shift” the bulk of the stream’s chemical energy into H<sub>2</sub>. The reaction taking place is:



This reaction is favored at low temperatures where the reaction rates are slow thus requiring the use of a sulfur-tolerant solid Co-Mo catalyst. To make the best use of the heat generated by the reaction and to adequately promote the formation of H<sub>2</sub> two shift reactors are employed in series with cooling in between either by pressurized steam generation or heating of boiler feed-water. The initial reactor converts 85-90% of the CO and allows the syngas to reach ~ 400°C by generating high pressure steam. Syngas then enters the second reactor where CO conversion proceeds adiabatically up to 98% and the temperature reaches 225°C. The syngas is again cooled as described earlier. A third low temperature reactor may be included for maximum conversion efficiencies of over 99% but is not always considered cost effective. Syngas is cooled at each stage in preparation for downstream processes.

- **Syngas conversion:** Pressure swing adsorption (PSA) units purify the hydrogen. High purity (~99.999%) H<sub>2</sub> is assumed to be extracted from the clean syngas at 35°C using PSA. As reviewed earlier, PSA units used in SMR operate at about 20 bar and reaches H<sub>2</sub> separation efficiencies in the range 85–90%. To maintain the same H<sub>2</sub> separation efficiency at pressures of 70 bar considered here would require a more complex (and more expensive) system arrangement and is consistent with current information. Pure hydrogen exits the PSA, while the purge gas (the remaining 15% H<sub>2</sub> along with the other species) is discharged at 1.5 bar and can be used to generate steam for power production in the steam turbine. At a pressure exceeding 60 bar, the H<sub>2</sub> product is suited for long-range pipeline transport and there is no need for further compression as with SMR. The larger and more complex PSA system required of gasification again is another parameter that results in it being more capital intensive over SMR.
- **Fuels and chemicals:** It was South Africa’s policy of apartheid and consequently economic sanctions being imposed that forced them to produce liquid fuels from hydrocarbon synthesis processes such as the Fisher-Tropsch method. This technology developed by German scientists during Hitler’s regime has been employed by Sasol successfully for the past 50 years. Gasification is the only advanced power generation technology capable of co-producing a wide variety of commodity and premium products (e.g., methanol, higher alcohols, diesel fuel, jet fuel and gasoline) in addition to hydrogen, electricity and industrial-grade process steam to meet future market requirements. It is this ability to produce value-added products from impure H<sub>2</sub>-rich syngas left after CO<sub>2</sub> removal that has made gasification economical in selected situations and will be a key driver in a deregulated power market. China maintains that shipping crude oil long distances from the coast to remote Inner Mongolia for conventional fuels refining would be expensive, whereas producing coal-derived fuels via liquefaction would be relatively competitive. Recently the Chinese government approved large-scale efforts to produce liquid

transportation fuels using coal gasification [12]. China's largest coal firm, Shenhua Group, plans to start up the country's first coal-to-fuels plant in 2007 or early 2008, in the world's most ambitious application of coal liquefaction since World War II. Shenhua plans to operate eight liquefaction plants by 2020, producing, in total, more than 30 million tons of synthetic oil annually - enough to displace more than 10 percent of her projected oil imports. China's progress in constructing coal-conversion plants puts it far ahead of the U.S., where coal gasification is still recovering from a damaged reputation. The finished fuels would be hauled from the plants in tank-cars via Shenhua's existing railroads adjacent to the mines. These trains already haul coal for later trans-shipment via waterways to city markets. To quantify the costs involved in producing such fuel pre-cursors is extremely case-specific and has not been considered in this analysis.

- **Fuel cells:** The most attractive energy conversion technology that uses hydrogen is fuel cells. A fuel cell is an energy conversion device that combines hydrogen and oxygen in an electrochemical process to produce a non fluctuating DC power output, some low-temperature heat, and water vapor as the only emissions. Different types of fuel cells are distinguished by their different electrolytes and the different temperatures reached during operation. Today, fuel cells are used in manned space flight to provide power for the spacecraft and drinking water for the astronauts; as backup power for critical services in hospitals and banks; and in an increasing number of cars and buses. Substantial development efforts are underway by automobile manufacturers in Germany, Japan and the U.S. to bring fuel cell vehicle technology to the market. Fuel cells such as POFC, SOFC and PEM cells are used today and will continue to increase in the future. Hydrogen fuel cell vehicles have several potential advantages over conventional gasoline engine vehicles including higher fuel efficiency, lower greenhouse gas and conventional pollutant emissions, longer lifetimes, and lower drive train maintenance costs. In addition, hydrogen fuel vehicles are projected to have excellent fuel economy at 66 mpg, gasoline equivalent [13]. If hydrogen produced with sequestration of the separated CO<sub>2</sub> were used in fuel cell cars, lifecycle CO<sub>2</sub> emissions per km would be less than 1/5 of those for gasoline internal combustion engine cars. Costs involved with the manufacture of fuel cells or the resulting drop in CO<sub>2</sub> emissions is beyond the scope of this analysis and has not been included.
- **Combustion/combustion turbine:** The cleaned synthesis gas is then combusted in a high efficiency gas turbine/generator to produce both electrical power and supply compressed air to the air separation unit that generates oxygen for the gasifier. The chemical energy of the low pressure PSA purge gas can be used to produce electric power. Due to the removal of CO<sub>2</sub> ahead of PSA the purge gas consists mainly of H<sub>2</sub> and its heating value is sufficiently high to justify its compression and its use as fuel in a combined cycle. The power generated can be increased by either by-passing more syngas over the PSA unit or by limiting the water-gas shift reaction. The separation of CO<sub>2</sub> however necessitates a higher steam requirement for dilution prior to shift conversion because of the higher heating values involved. The generation of gas turbine used for these systems are typically the steam cooled GE 107H or the Siemens V64.3a that offer significant efficiency gains and cost reduction. As mentioned previously, in order to limit NO<sub>x</sub> emissions, N<sub>2</sub> from the air separator is compressed and injected into the combustor [14]. The costs for the selected gas turbine are included in the capital costs developed.



- Heat recovery steam generator (HRSG) and steam turbine:** The hot combustion gas from the turbine is sent to a HRSG, which in turn, drives a steam turbine/generator to produce additional electrical power. In this mode of operation, a major portion of the electricity required is produced in the combustion gas turbine/generator. The steam cycle that bottoms the gas turbine is highly integrated with the gasification process, which, depending on the plant scheme, provides heat for evaporation, high pressure superheat (in the syngas cooler) and feed-water heating. Re-heat and low pressure superheat are generated at the HRSG.

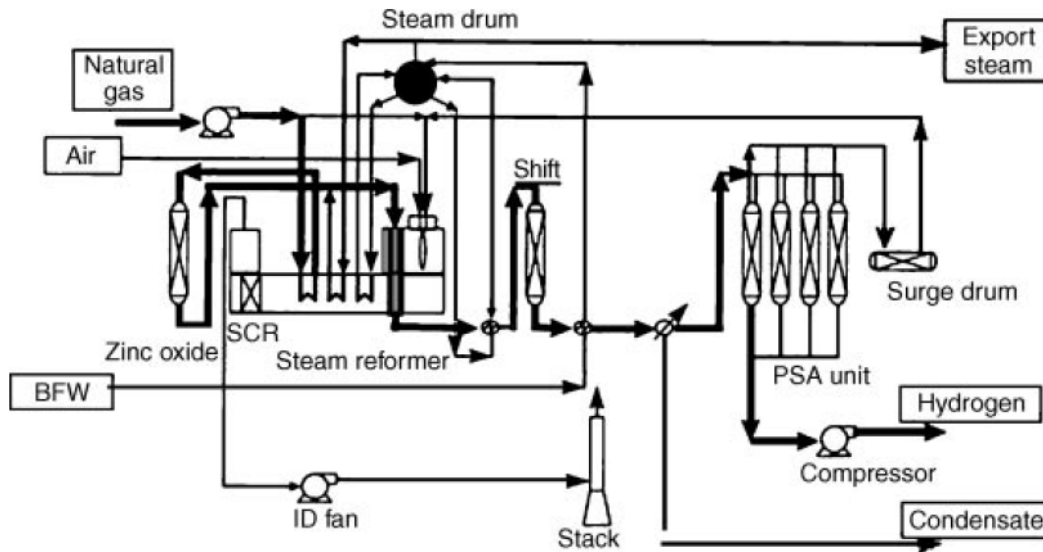


Figure 2-1. Simplified Block Diagram of SMR

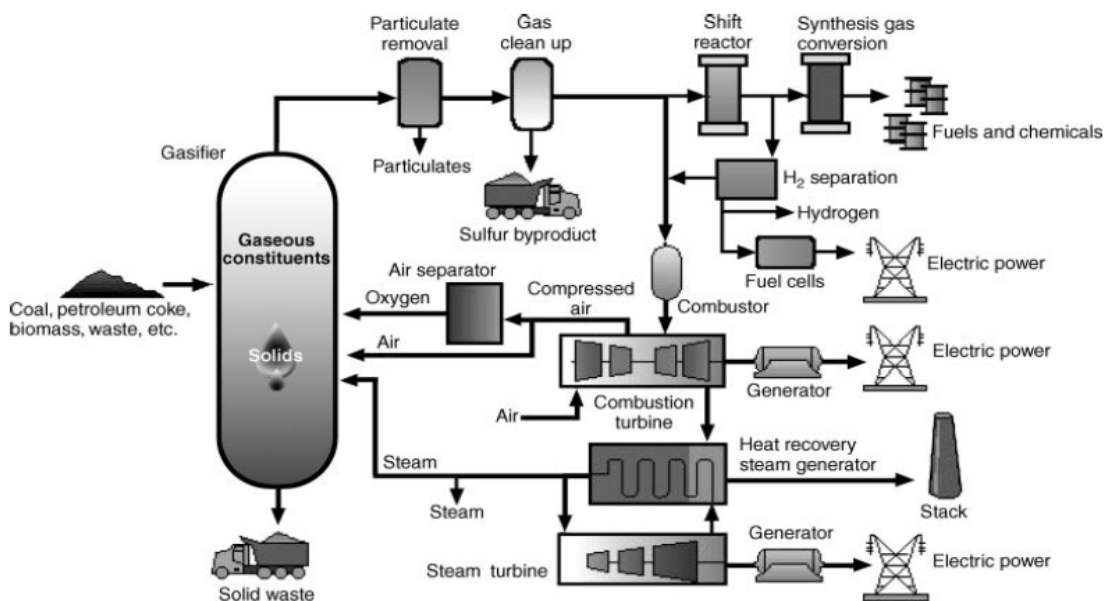


Figure 2-2. Detailed Process Flow Diagram of Gasification

## CHAPTER 3 ECONOMIC ANALYSIS

### **3.1 Methodology**

This analysis is kept simple and transparent to facilitate revision by readers wishing to use different economic assumptions. To decide if a given process is a good investment as opposed to another:

- Capital Cost must be determined.
- Operating Cost or Cost of Manufacturing must be determined.
- A comparison must be made of certain parameters which will be defined in this chapter.

These parameters are determined by combining the capital and operating costs.

The Chemical Engineering Plant Cost Index (CEPCI) has been employed to calculate all costs as per 2006 \$ value. Using the more common consumer price index (CPI) issued by the U.S. government is not accurate. This index represents a composite cost index that reflects changing costs due to inflation for the average consumer of a number of goods (e.g. housing, cost of basic foods, transportation etc.); these are weighted appropriately to reach a value reflecting the average cost of these goods and hence cannot be used. The basis for this cost index is shown in Table 3-1.

### **3.2 Capital Cost Estimate**

Capital cost pertains to the costs associated with the construction of a new plant. These capital costs are based on equipment module costing techniques developed by Guthrie [15] in the early 1970s and forms the basis of many of the equipment module techniques in use today. This costing technique relates all costs back to the purchased cost of equipment evaluated for some base conditions. Deviations from these base conditions are handled by using multiplying factors that depend on the specific equipment, pressure and materials of construction.

To determine the capital cost for both technologies would require a detailed analysis of each component and is beyond the scope of this work. For both SMR and gasification, the capital cost developed by Basye et al. [16] are updated to 2006 \$ and used as a base value to which further costs are added. The costs of each included component will be mentioned as and when they are included.

The final capital cost estimates developed for both SMR and gasification will henceforth be referred to as Fixed Capital Investment without including the cost of land ( $FCI_L$ ). The cost of land is not included as part of FCI since it is considered an investment that cannot be depreciated since it is recoverable at the end of the project life. Since the primary aim of this economic analysis is a comparison of SMR and gasification the cost of land is assumed to be of the same order and is therefore neglected.

### **3.3 Operating Cost or Cost of Manufacturing Estimate (COM)**

The more important factors that influence the cost of manufacturing are provided along with a brief explanation of each. The approach provided to calculate COM is similar to that expressed in most engineering practices that have been well established for several decades and is explained in detail below [17]. They can be broadly classified into three categories:

- 1. Direct manufacturing costs:** These costs represent operating expenses that vary with production rate. The formulae represented here are in keeping with the model developed, but have been modified in certain cases for a more realistic approach.
- **Raw materials ( $C_{RM}$ ):** The raw materials used for SMR and gasification are natural gas and coal. The industrial price of natural gas in 2006 as per the EIA was \$7.5/GJ. The price of coal used, \$1.45/GJ (based on the higher heating value) was the average cost to U.S. electric generators in 2006 as per the U.S. Energy Information Agency. Hydrogen production capacities are obtained from Bayse et al [16]. Process efficiencies have been updated according to recently published data [18]. Final  $C_{RM}$  values are presented in the appendix.
- **Waste treatment ( $C_{WT}$ ):** The cost of waste treatment is assumed to be zero and not factored into the Cost of Manufacturing, but the equipment used (e.g. desulfurizer, Selexol system used for  $CO_2$  removal etc.) are accounted for while calculating  $FCI_L$ .

- **Utilities ( $C_{UT}$ ):** Costs of utility streams are determined according to the requirements of equipment used.  $C_{UT}$  is difficult to estimate because of fluctuations that arise owing to geographic and political variations.  $C_{UT}$  for both SMR and gasification has been updated from previously published work [19]. Cost of process water has been included for both methods and is presented in the appendix. The huge difference between the two is a result of the maintenance and process water requirements.
- **Operating labor ( $C_{OL}$ ):** Cost of personnel required for plant operations. The technique used to estimate operating labor requirements is based on a correlation developed by Alkhatat and Gerrard [20]. According to this method the operating labor requirement is given by the equation:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23 N_{np})^{0.5} \quad (3-1)$$

where  $N_{OL}$  is the number of operators per shift,  $P$  is the number of processing steps that involve handling, transportation and distribution, particle size control and removal.  $N_{np}$  is the number of non-particulate processing steps and includes compression, heating and cooling, mixing and reaction. A single operator works on the average 49 weeks a year, at 5, 8-hour shifts per week. This amounts to 245 shifts/operator per year and assuming 3, 8-hour shifts per day we have 1,095 operating shifts per year. Hence the number of operators needed to provide for 1,095 shifts per year would be 4.5. Since  $N_{OL}$  gives the number of operators per shift per year, this number should be multiplied by 4.5 and rounded off to the nearest whole number to determine the number of operators that need to be hired. From the U.S. Bureau of Labor and Statistics the annual wages for a chemical manufacturing facility is \$19/hour which can be rounded off to \$40,000 per year for 2,000 hours per year. Hence multiplying the above number by \$40,000 results in  $C_{OL}$ . The results of the final  $C_{OL}$  are presented in the appendix.

- **Direct supervisory and clerical labor:** Cost of administrative/engineering and support personnel. This cost can be expressed in terms of  $C_{OL}$  as  $(0.18) C_{OL}$ .
- **Maintenance and repairs:** Cost of labor and materials associated with maintenance. This cost can be expressed as  $(0.06) FCI_L$ .
- **Operating Supplies:** Cost of miscellaneous supplies that support daily operation are not considered to be raw materials. Examples include lubricants, filters, respirators and protective equipment for operators etc. The cost of operating supplies is  $(0.009) FCI_L$ .
- **Laboratory charges:** Costs of routine and special laboratory tests required for product quality control and testing. These charges are represented as  $(0.15) FCI_L$ .
- **Patents:** Cost of using patented or licensed technology. Patents are accounted for as  $(0.03) COM$ .

Therefore the Total Direct Manufacturing Costs can be written as  $C_{RM} + C_{WT} + C_{UT} + 1.33 C_{OL} +$

$$0.03 \text{ COM} + 0.069 \text{ FCI}_L$$

**2. Fixed manufacturing costs:** Factors not affected by the level of production. These costs occur even when the plant is not in operation.

- **Depreciation:** Costs associated with the physical plant (buildings, equipment etc.). According to published data a 10% depreciation is adopted. Therefore depreciation is  $(0.1) \text{ FCI}_L$ . As will be seen towards the end of this section this is just a crude approximation to eliminate depreciation and is discussed separately owing to its significance in calculating cash flows.
- **Local taxes and insurance:** Costs associated with property taxes and liability insurance. Based on plant location and risks associated with the process and is expressed as  $(0.032) \text{ FCI}_L$ .
- **Plant overhead costs:** Includes all costs associated with operations of auxiliary facilities supporting the manufacturing process. Costs involve payroll and accounting services, fire protection and safety, medical services, cafeteria and recreation facilities, payroll overhead and employee benefits. These can be expressed as  $(0.708) \text{ C}_{OL} + (0.036) \text{ FCI}_L$ .

Therefore the Total Fixed Manufacturing Costs can be written as  $(0.708) \text{ C}_{OL} + (0.068) \text{ FCI}_L +$  depreciation.

**3. General expenses:** These costs represent an overhead burden that is necessary to carry out business functions. They include management, sales, financing, and research expenses. These seldom vary with production however in some cases research expenses do increase with an increase in production.

- **Administration costs:** Costs for administration; includes salaries, other administration, buildings and other related activities. Administration costs are  $(0.177) \text{ C}_{OL} + (0.009) \text{ FCI}_L$ .
- **Distribution and selling costs:** Costs of sales and marketing required to sell chemical products. Includes salaries and other miscellaneous costs. Distribution and selling costs amount to  $(0.011) \text{ COM}$ .
- **Research and development:** Costs of research activities related to the product. Includes salaries and funds for research related equipment and supplies. R&D costs are represented as  $(0.05) \text{ COM}$ .

Therefore the Total General Manufacturing Costs can be written as  $(0.177) \text{ C}_{OL} +$

$$(0.009) FCI_L + (0.16) COM.$$

Finally Total Cost of Manufacturing,

$$COM = (0.28) FCI_L + (2.73) C_{OL} + (1.23) (C_{UT} + C_{WT} + C_{RM})$$

At this point a mention should be made that  $COM_d = COM - \text{depreciation} = (0.18) FCI_L + (2.73) C_{OL} + (1.23) (C_{UT} + C_{WT} + C_{RM})$ . This will be useful when describing the policy adopted to calculate the cash flows generated for both processes in the following section.

### 3.4 Steps to Compare Economic Merit

To be able to judge the economic merit of SMR and gasification,  $FCI_L$  and  $COM_d$  must be combined and compared. This is explained further.

- 1. Cash flow:** Cumulative cash flow diagrams that incorporate time value of money are an effective way to analyze inflow and outflow of money. Different methods of comparisons of SMR and gasification that are outlined here can only be derived based on creating cash flow diagrams. Each component required to generate a cash flow diagram will now be discussed briefly with only required information presented to simplify the analysis. Calculated results are presented in the appendix.
- **Fixed Capital Investment without the cost of land,  $FCI_L$ :** Capital Cost is considered as fixed capital i.e. capital which cannot be recovered at the end of the plant life. Hence in order to calculate depreciation (which is an integral part of any cash flow), we first determine  $FCI_L$  which is the fixed capital excluding the cost of land. The cost of land is not included since it is the only part of the fixed capital investment that cannot be depreciated or is recoverable at the end of the plant's life. In all analyses the fixed capital which is incurred at the beginning of the life of a plant will be expressed spread over a period of time. A construction life of three years is assumed for both SMR and gasification and the  $FCI_L$  is spread at 10%, 35% and 55% respectively at the end of each year.
- **Taxation, (t):** Taxation has a direct impact on the profits realized from building and operating a plant. When comparing projects, the effect of taxes must always be accounted for. Taxation rates for companies and the laws governing taxation change frequently. For most large corporations, the basic federal taxation rate is 35%. In addition corporations must also pay state, city and other local taxes. The overall taxation rate is often in the range of 40% to 50% as per the Federal Tax Rate Schedule for Corporations in 2001 [21]. A tax rate of 42% is assumed for this study.

- **Interest rate, (i):** An annual interest rate of 10% has been assumed. Denoted as (i), the interest is factored while computed discounted cash flows. This “internal” interest rate is usually determined by corporate management and represents the minimum acceptable rate of return that any company will accept for any new investment.
- **Working Capital:** Working capital comprises of variables defined earlier -  $C_{RM}$ ,  $FCI_L$  and  $C_{OL}$ . A factor of 10% for each component adds up to the working capital as shown:

$$\text{Working Capital} = (0.10) C_{RM} + (0.10) FCI_L + (0.10) C_{OL}$$

- **Salvage, (S):** Salvage is the scrap value of the plant equipment at the end of its useful life. Salvage value for equipment is typically zero; however a salvage of 10% of  $FCI_L$  is estimated conservatively for both methods since a plant life of 20 years has been set (see below), which is lower than the typical life for a project of this magnitude.
- **Revenue, (R):** Revenue generated from both plants are computed and presented in the appendix. Revenue is generated only after construction period of the plant in this case, after 3 years and is assumed to be constant over the plant life. For both plants a hydrogen production capacity of 11,870,000 GJ has been assumed as described earlier. Literature regarding the costs of hydrogen produced by SMR and gasification were obtained from two detailed estimates [22, and 23]. All sources reached a price of approximately \$5 - \$8/GJ for a 1994 \$ value for SMR and the price of hydrogen produced by gasification was calculated to be in the range of about \$10 - \$12/GJ, 1994 \$ value.

For this analysis the cost of hydrogen generated as revenue was varied to determine the least positive NPV for either project to break even. As shown in Figure 3-1 the lowest cost of hydrogen produced by SMR (\$15.5/GJ) was much lower than that of gasification (~ \$20/GJ). These values agree with the detailed studies mentioned where costs of hydrogen produced from SMR and gasification can be scaled to a 2006 \$ value of \$11/GJ and \$16/GJ respectively. More recent studies show that the hydrogen selling price by gasification can be reduced further by the added benefits of revenue generated from other valuable by-products such as fuel pre-cursors, industrial grade steam and electricity which have not been accounted for here.

Hence for a more thorough comparison the price of hydrogen generated will be assumed as \$21/GJ for both SMR and gasification.

- **Cost of Manufacturing with depreciation, ( $COM_d$ ):**  $COM_d$  is the cost of manufacturing excluding depreciation and is calculated based on relevant information provided earlier.
- **Plant life, (n):** The plant life indicates the life of the plant equipment to be used in calculations. Since both SMR and gasification plants are capital intensive processes, the plant life will henceforth be assumed as 20 years according to the guidelines set by the U.S. Department of Treasury [24].
- **Depreciation:** Depreciation is defined as the difference between the original cost and the salvage value. Only fixed capital can depreciate. Working capital (salaries, raw material,

contingencies) is recoverable at the end of the plant's life and is not depreciated. Depreciation is normally dependent on location of the plant. Contrary to most similar analyses performed where either the Straight Line method (SL) or Double Declining Balance (DDB) (both approved by the U.S. Internal Revenue Service (IRS)) is adopted for simplicity, the Modified Accelerated Cost Recovery System (MACRS) has been adopted for this purpose. The current federal tax law is based on MACRS and uses a half-year convention. Since the plant and equipment life for this analysis has been set at 20 years the MACRS here will be used over a shorter period of time, which is 10 years for this class life. This method ensures greater accuracy since it is better to depreciate an investment as early as possible to allow less tax paid in a given year. The MACRS method uses the DDB method and switches to the SL method when the latter yields a greater depreciation allowance for that year. The half-year convention assumes that the equipment is bought midway through the first year for which depreciation is allowed and so the first year depreciation is only half of that for a full year. Likewise in the eleventh (and last) year after the 3-year construction period, the depreciation is again for one-half year. The MACRS generally follows this pattern since DDB method has the largest depreciation in the early years and SL method represents the largest depreciation towards the end of the project life. Both SL and DDB methods are described briefly:

- i. Straight Line depreciation method - In this method an equal amount of depreciation is charged each year over the depreciation period allowed. The annual depreciation in a certain year,  $k$  is denoted as  $d_k$ . The total capital for depreciation,  $D = FCI_L - S$ .

$$d_k = D / n \quad (3-2)$$

- ii. Double Declining Balance method of depreciation - In this method the amount of depreciation each year is a constant fraction (here 2) of the book value,  $BV_{k-1}$ .

$$d_k^{DDB} = \frac{2}{n} \left[ FCI_L - \sum_{j=0}^{j=k-1} d_j \right] \quad (3-3)$$

- **After tax cash flow:** The cash flow after taxes is finally calculated as the sum of the net profit after taxes and depreciation.

$$\text{After tax cash flow} = \text{Net profit} + \text{Depreciation} = (R - COM_d - d_k) (1-t) + d_k \quad (3-4)$$

- **Cumulative discounted cash flow:** Finally the cumulative discounted cash flows are computed based on the discounted cash flows for each year. An annual interest rate of 10% is used.

$$\text{Discounted cash flow} = \frac{\text{After tax cash flow}}{[(1+i)^n]} \quad (3-5)$$

Results are presented in Chapter 4.



- 2. Comparison parameters:** Certain parameters that will be useful in comparing the economic merit of both projects will now be discussed. All parameters are discounted back to the initial start-up time of the project to account for the time value of money. Using non-discounted techniques to evaluate the profitability of projects of this magnitude and level of investment is not recommended. The discounted parameters used in this analysis can be broadly classified into three criteria: cash, time, and interest, and are explained further in this section:
- **Net Present Value (NPV):** Cumulative discounted cash position at the end of the project life. Values greater than unity indicate profitable processes while those less than unity represent unprofitable projects. A higher NPV is always more desirable. The NPV of a project is the final cumulative discounted cash value at the end of the project life.
  - **Discounted Payback period (DPBP):** Time required after start-up to recover the  $FCI_L$  required for the project with all cash flows discounted back to the initial time. To determine the DPBP, the working capital is discounted back in time and the number of years required after the project construction period to recover this amount equals the DPBP. The project with a shorter payback period is considered more desirable.
  - **Discounted Cash Flow Rate of Return (DCFROR):** Interest rate at which all the cash flows must be discounted in order for the NPV of the project to equal zero. In other words, DCFROR represents the highest, after-tax interest or discount rate at which the project can just break even. If the DCFROR calculated for a project is greater than the internal discount rate (here assumed 10%) then it is considered profitable. There are two methods of calculating the DCFROR, either iteratively determine the value of “i” for which NPV equals zero or solve the equation for NPV expressed in terms of “i” as the sum of the cumulative discounted cash value at the end of each year.
  - **Monte-Carlo Simulation:** The Monte-Carlo method is a concept of assigning probability distributions to parameters, repeatedly choosing variables from these distributions and using these values to calculate a function dependent on the variables. As a result a sensitivity analysis arising due to risk and demand can be quantified graphically for PBP, NPV and ROR and are presented in Chapter 4. According to Humphrey [25], parameters that are normally varied and their probability distributions have been presented in Table 3-2.

However since the goal of this study is a comparison of SMR and gasification the approach as shown above will have to be modified to produce satisfactory results. The only real parameter that can be varied in this situation is the Cost of Raw Material,  $C_{RM}$ . To produce realistic results a real-time analysis was performed of the variation of the costs of both imported natural gas and domestically available coal from 1985 to 2005, as reported by the EIA. A twenty-year period was chosen in keeping with the assumed 20 year construction period for both projects and the year 1995 was selected as the baseline for price variation. Forecasts of prices were not used to preserve the accuracy. As is evident from Figure 3-2, the percentage variation of the price of natural gas is far greater than that of coal. Hence the variations in  $C_{RM}$  that have been used for the Monte Carlo simulation are in keeping with the results presented above and are presented in Table 3-3.

As explained above each parameter is chosen and a random variable is selected from within the probability distribution range. Corresponding values of NPV, DCFROR and DPBP are determined using the calculated values at a hydrogen selling price of \$21/GJ as the base value. These steps are then repeated; (the more values obtained the smoother the curve). Cumulative probability data are then determined and then plotted. The results of the Monte Carlo simulation are presented in Chapter 4.

Table 3-1. Basis for the Chemical Engineering Plant Cost Index

| Components of index                            | Weighing of component (%) |              |
|--|---------------------------|--------------|
| Equipment, machinery, and support              |                           |              |
| (a) Fabricated equipment                       | 37                        |              |
| (b) Process machinery                          | 14                        |              |
| (c) Pipe, valves and fittings                  | 20                        |              |
| (d) Process instruments and controls           | 7                         |              |
| (e) Pumps and compressors                      | 7                         |              |
| (f) Electrical equipment and materials         | 5                         |              |
| (g) Structural supports, insulation, and paint | 10                        |              |
|  | 100                       | 61% of total |
| Erection and installation labor                |                           | 22           |
| Buildings, materials and labor                 |                           | 7            |
| Engineering and supervision                    |                           | 10           |
| Total  |                           | 100          |

The CEPCI for 2006 is 478.7 and will be used for all calculations henceforth.

Table 3-2. Probable Variation of Key Parameters

| Parameter                             | Lower limit | Upper limit |
|---------------------------------------|-------------|-------------|
| FCI <sub>L</sub>                      | - 20%       | 30%         |
| Price of hydrogen                     | - 10%       | 10%         |
| Working capital                       | - 50%       | 10%         |
| Income tax rate, t                    | - 20%       | 20%         |
| Interest rate, i                      | - 10%       | 20%         |
| Cost of raw material, C <sub>RM</sub> | - 20%       | 20%         |
| Salvage value, S                      | - 80%       | 20%         |

Table 3-3. Probable Variation of Cost of Raw Material: C<sub>RM</sub>

| Parameter                             | Steam Methane Reformation (SMR) |             | Gasification |             |
|---------------------------------------|---------------------------------|-------------|--------------|-------------|
|                                       | Lower limit                     | Upper limit | Lower limit  | Upper limit |
| Cost of raw material, C <sub>RM</sub> | 0 %                             | 445 %       | - 17.9 %     | 76.9 %      |

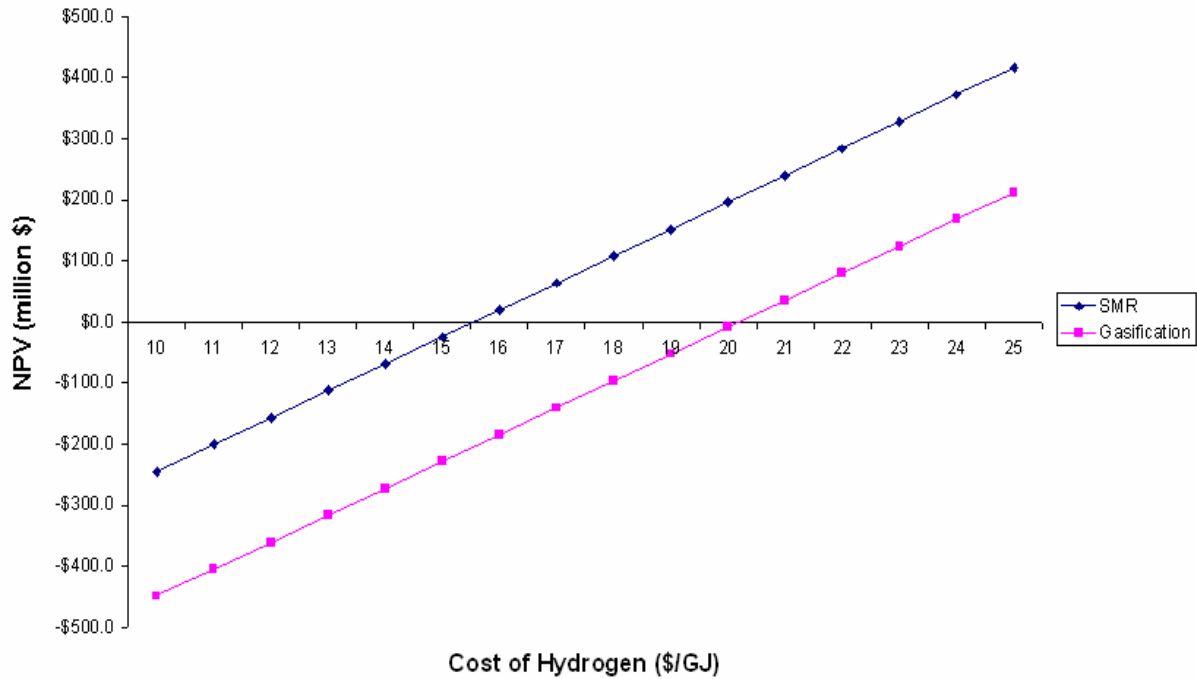


Figure 3-1. Hydrogen Price Analysis with Net Present Value (NPV)

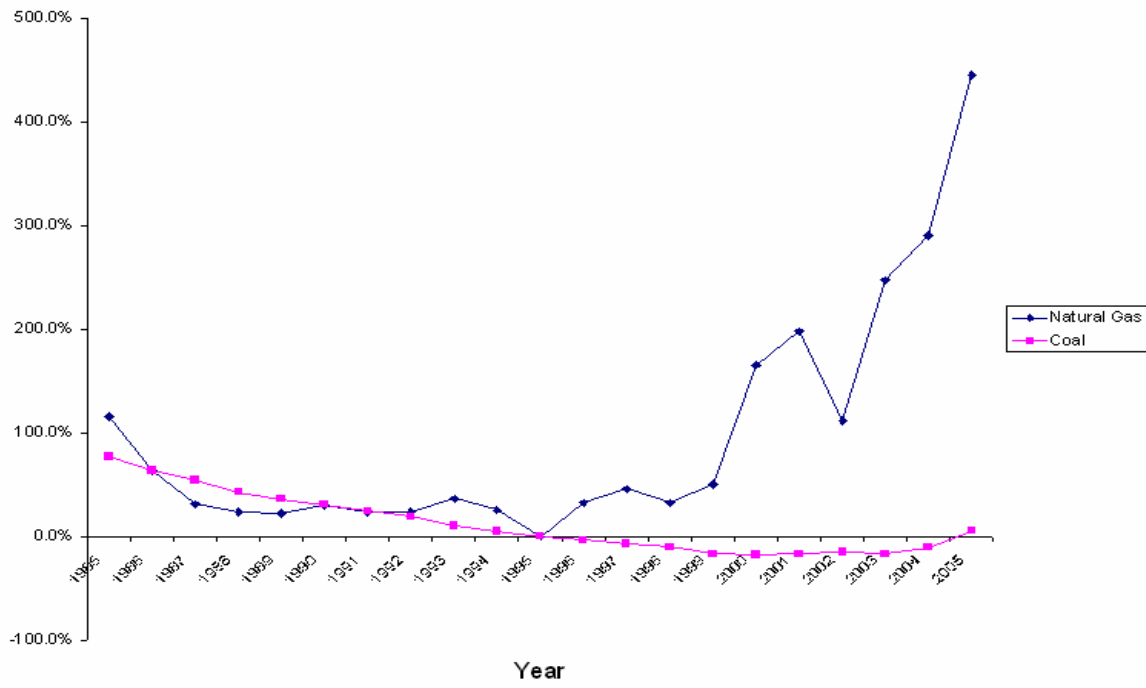


Figure 3-2. Fluctuation in Price of Natural Gas and Coal (1985-2005)

## CHAPTER 4 RESULTS AND DISCUSSION

This paper serves to examine the economic ramifications of two methods of hydrogen production: one that is commercially already in existence worldwide, SMR; and the other which has begun to gain a lot of interest among governments worldwide-Gasification.

Although gasification is a well-established technology, it can only be competitive with SMR when coal is available in plenty (e.g. U.S., China, and India). Increase in prices can be attributed to various reasons-increased costs due to handling and pre-treatment of coal, increased water requirements, more capital intensive equipment required for heavier cleanup operations and labor requirements among others.

However in spite of being much more expensive, it still enjoys widespread popularity because Integrated Gasification Combined Cycle power generation systems have shown considerable potential for producing chemicals apart from hydrogen - products include ammonia, methanol and synthetic natural gas, and conventional transportation fuels [35]. This substantially reduces the overall cost, improves system efficiency and reduces emissions. Because there are significant coal reserves in many areas of the world, coal could replace natural gas and oil as the primary feedstock for hydrogen production in those areas and one day promote energy independence for those nations.

The results of the economic analysis will now be presented as explained in Chapter 3. As is evident from Figure 4-1 and Table 4-3 (and in agreement with published data) SMR is the commercially preferred option, with a higher NPV, higher DCFROR and lower payback period. Next, the results of the Monte-Carlo risk simulation are presented for NPV, DCFROR and DPBP (Figures 4-2, 4-3 and 4-4).

The results show that for a cumulative probability of 500 (the median probability value situation) the NPV of gasification is higher than SMR. Although both SMR and gasification show high probability to reach their respective values of NPV as calculated, there is still a

high enough probability that indicates that the risks associated with SMR are high. Figure 4-3 proves that the probability of SMR having a decent DCFROR is low. In comparison gasification shows a much stronger probability of attaining a higher DCFROR than SMR. The results from Figure 4-4 are similar to Figure 4-3. While SMR shows a low probability of a decent payback period, the probability of a payback period of nearly 20 years is much higher in the case of gasification.

The above results are a strong indicator that despite the fact that current results show that SMR may be a cheaper option, the risks associated are high and warrant massive investment in gasification - the technology of the future.

Table 4-1. Discounted Cash Flow Diagram for Steam Methane Reformation (SMR)

| Year | Investment<br>(million \$) | Depreciation<br>$d_k$<br>(million \$) | $FCI_L - Sd_k$<br>(million \$) | Revenue<br>$R$<br>(million \$) | $COM_d$<br>(million \$) | $(R - COM_d - d_k)(1-t) + d_k$<br>(million \$) | Cash flow<br>(non-<br>discounted)<br>(million \$) | Cash flow<br>(discounted)<br>(million \$) | Cumulative cash flow<br>(discounted)<br>(million \$) |
|------|----------------------------|---------------------------------------|--------------------------------|--------------------------------|-------------------------|--|---|---|--|
| 0    | 0.00                       |                                       | 136.10                         |                                |                         |  | 0.00  | 0.00                                      | 0.00   |
| 0    | 0.00                       |                                       | 136.10                         |                                |                         |  | 0.00  | 0.00                                      | 0.00   |
| 1    | 13.61                      |                                       | 136.10                         |                                |                         |  | (13.61)   | (12.37)                                   | (12.37)  |
| 2    | 47.64                      |                                       | 136.10                         |                                |                         |  | (47.64)   | (39.37)                                   | (51.74)  |
| 3    | 74.86                      |                                       | 136.10                         |                                |                         |  | (74.86)   | (56.24)                                   | (107.98)   |
| 3    | 24.20                      |                                       | 136.10                         |                                |                         |  | (24.20)   | (18.18)                                   | (126.16)   |
| 4    |                            | 13.61                                 | 122.49                         | 249.27                         | 159.10                  | 58.02  | 58.02   | 39.63                                     | (86.54)  |
| 5    |                            | 24.50                                 | 97.99                          | 249.27                         | 159.10                  | 62.59  | 62.59   | 38.86                                     | (47.67)  |
| 6    |                            | 19.60                                 | 78.39                          | 249.27                         | 159.10                  | 60.53  | 60.53   | 34.17                                     | (13.50)  |
| 7    |                            | 15.65                                 | 62.74                          | 249.27                         | 159.10                  | 58.87  | 58.87   | 30.21                                     | 16.71  |
| 8    |                            | 12.52                                 | 50.22                          | 249.27                         | 159.10                  | 57.56  | 57.56   | 26.85                                     | 43.56  |
| 9    |                            | 10.07                                 | 40.15                          | 249.27                         | 159.10                  | 56.53  | 56.53   | 23.97                                     | 67.53  |
| 10   |                            | 8.98                                  | 31.17                          | 249.27                         | 159.10                  | 56.07  | 56.07   | 21.62                                     | 89.15  |
| 11   |                            | 8.98                                  | 22.18                          | 249.27                         | 159.10                  | 56.07  | 56.07   | 19.65                                     | 108.81   |
| 12   |                            | 8.85                                  | 13.34                          | 249.27                         | 159.10                  | 56.02  | 56.02   | 17.85                                     | 126.65   |
| 13   |                            | 8.85                                  | 4.49                           | 249.27                         | 159.10                  | 56.02  | 56.02   | 16.23                                     | 142.88   |
| 14   |                            | 4.49                                  | -                              | 249.27                         | 159.10                  | 54.19  | 54.19   | 14.27                                     | 157.15   |
| 15   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 12.52                                     | 169.67   |
| 16   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 11.38                                     | 181.05   |
| 17   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 10.35                                     | 191.40   |
| 18   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 9.41                                      | 200.81   |
| 19   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 8.55                                      | 209.36   |
| 20   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 7.77                                      | 217.13   |
| 21   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 7.07                                      | 224.20   |
| 22   |                            |                                       | -                              | 249.27                         | 159.10                  | 52.30  | 52.30   | 6.42                                      | 230.62   |
| 23   |                            |                                       | -                              | 249.27                         | 159.10                  | 60.19  | 60.19   | 6.72                                      | 237.35   |
| 23   |                            |                                       |                                |                                |                         |  | 24.20   | 2.70                                      | 240.05   |

Table 4-2. Discounted Cash Flow Diagram for Gasification

| Year | Investment<br>(million \$) | $d_k$<br>(million \$) | $FCI_L - Sd_k$<br>(million \$) | Revenue<br>R<br>(million \$) | $COM_d$<br>(million \$) | $(R - COM_d - d_k)(1-t) + d_k$<br>(million \$) | Cash flow<br>(non-<br>discounted)<br>(million \$) | Cash flow<br>(discounted)<br>(million \$) | Cumulative cash flow<br>(discounted)<br>(million \$) |
|------|----------------------------|-----------------------|--------------------------------|------------------------------|-------------------------|--|---|---|--|
| 0    | 0.00                       |                       | 535.90                         |                              |                         |  | 0.00  | 0.00                                      | 0.00   |
| 0    | 0.00                       |                       | 535.90                         |                              |                         |  | 0.00  | 0.00                                      | 0.00   |
| 1    | 53.59                      |                       | 535.90                         |                              |                         |  | (53.59)   | (48.72)                                   | (48.72)  |
| 2    | 187.57                     |                       | 535.90                         |                              |                         |  | (187.57)  | (155.01)                                  | (203.73)   |
| 3    | 294.75                     |                       | 535.90                         |                              |                         |  | (294.75)  | (221.45)                                  | (425.18)   |
| 3    | 56.73                      |                       | 535.90                         |                              |                         |  | (56.73)   | (42.62)                                   | (467.80)   |
| 4    |                            | 53.59                 | 482.31                         | 249.27                       | 145.97                  | 82.42  | 82.42   | 56.29                                     | (411.50)   |
| 5    |                            | 96.46                 | 385.85                         | 249.27                       | 145.97                  | 100.43   | 100.43  | 62.36                                     | (349.14)   |
| 6    |                            | 77.17                 | 308.68                         | 249.27                       | 145.97                  | 92.32  | 92.32   | 52.11                                     | (297.03)   |
| 7    |                            | 61.63                 | 247.05                         | 249.27                       | 145.97                  | 85.80  | 85.80   | 44.03                                     | (253.00)   |
| 8    |                            | 49.30                 | 197.75                         | 249.27                       | 145.97                  | 80.62  | 80.62   | 37.61                                     | (215.39)   |
| 9    |                            | 39.66                 | 158.09                         | 249.27                       | 145.97                  | 76.57  | 76.57   | 32.47                                     | (182.92)   |
| 10   |                            | 35.37                 | 122.72                         | 249.27                       | 145.97                  | 74.77  | 74.77   | 28.83                                     | (154.10)   |
| 11   |                            | 35.37                 | 87.35                          | 249.27                       | 145.97                  | 74.77  | 74.77   | 26.21                                     | (127.89)   |
| 12   |                            | 34.83                 | 52.52                          | 249.27                       | 145.97                  | 74.54  | 74.54   | 23.75                                     | (104.14)   |
| 13   |                            | 34.83                 | 17.68                          | 249.27                       | 145.97                  | 74.54  | 74.54   | 21.59                                     | (82.55)  |
| 14   |                            | 17.68                 | -                              | 249.27                       | 145.97                  | 67.34  | 67.34   | 17.73                                     | (64.81)  |
| 15   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 14.34                                     | (50.47)  |
| 16   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 13.04                                     | (37.43)  |
| 17   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 11.85                                     | (25.58)  |
| 18   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 10.78                                     | (14.80)  |
| 19   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 9.80                                      | (5.01)   |
| 20   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 8.91                                      | 3.90   |
| 21   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 8.10                                      | 12.00  |
| 22   |                            |                       | -                              | 249.27                       | 145.97                  | 59.91  | 59.91   | 7.36                                      | 19.36  |
| 23   |                            |                       | -                              | 249.27                       | 145.97                  | 90.99  | 90.99   | 10.16                                     | 29.52  |
| 23   |                            |                       |                                |                              |                         |  | 56.73   | 6.34                                      | 35.85  |



Table 4-3. Discounted Profitability Criteria for Steam Methane Reformation (SMR) and Gasification

| Project      | Net present value (NPV) (million \$) | Discounted cash flow rate of return (DCFROR) (%) | Discounted payback period (DPBP) (years) |
|--------------|--------------------------------------|--|--|
| SMR          | 240.1                                | 31.5   | 2.9                                      |
| Gasification | 35.9                                 | 11.1   | 12.6                                     |

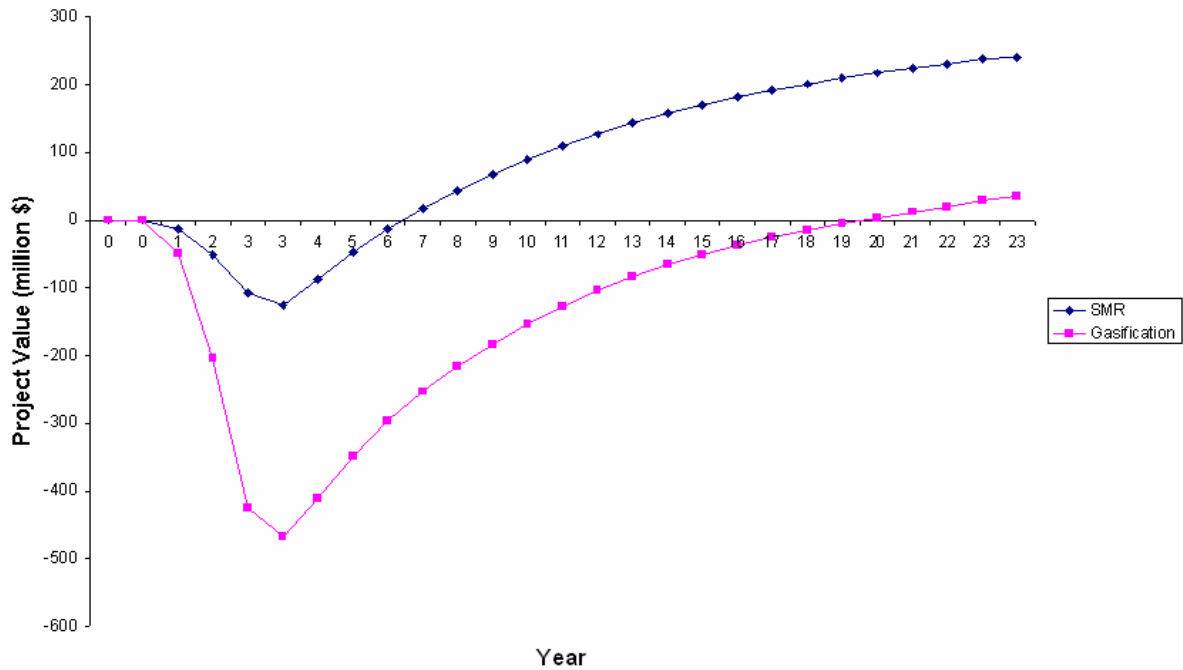


Figure 4-1. Discounted Cash Flow Diagram for SMR and Gasification

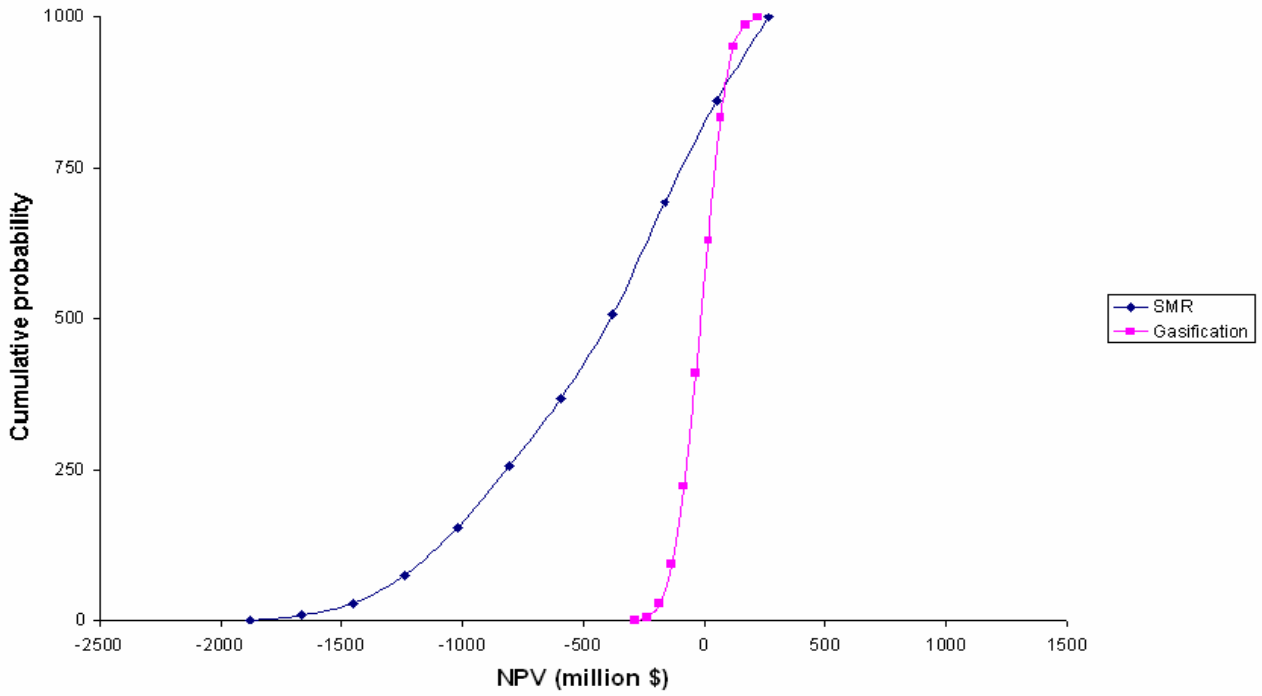


Figure 4-2. Probability Distribution: Net Present Value (NPV)

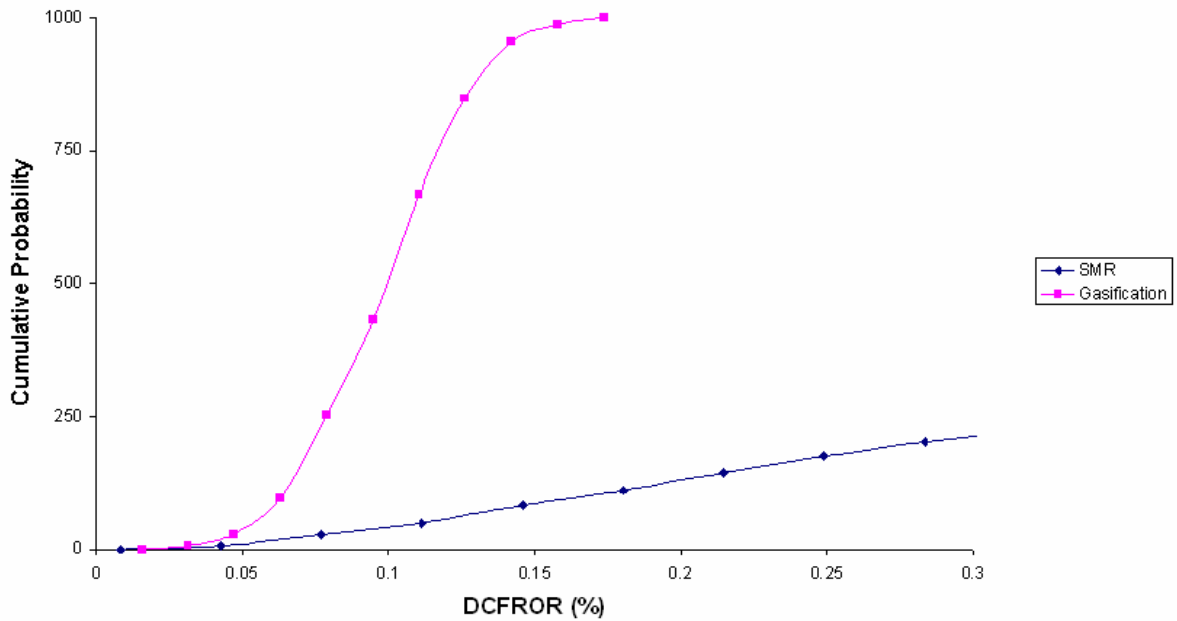


Figure 4-3. Probability Distribution: Discounted Cash Flow Rate of Return (DCFROR)

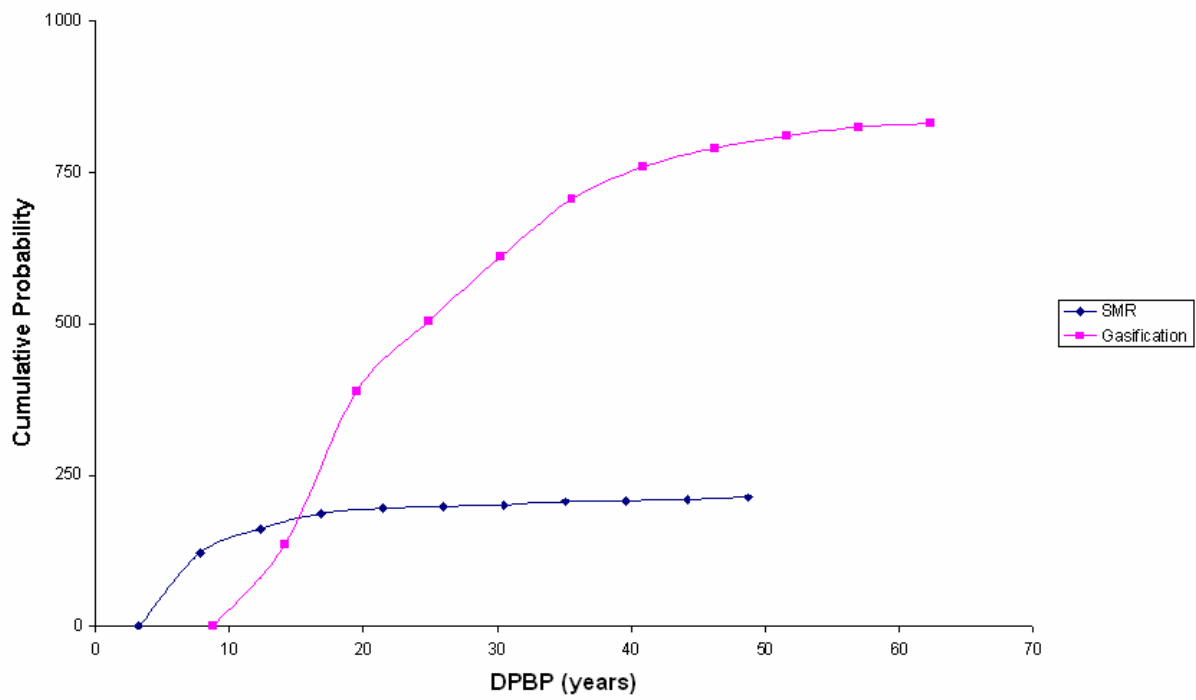


Figure 4-4. Probability Distribution: Discounted Payback Period (DPBP)

## CHAPTER 5 CONCLUSIONS

Our study showed that in the future gasification could prove to be the more attractive alternative when compared to SMR for hydrogen production. This is evident from the following:

- The NPV of gasification is \$36 million while that of SMR is \$240 million. This indicates that the net value of the project is significantly higher for SMR.
- The DCFROR for gasification 11% while that of SMR is 32%. Since we have assumed an internal rate of return as 10% it is evident that while both projects are viable, SMR is a superior alternative.
- Gasification has a DPBP of 12.6 years whereas that of SMR is 2.9 years.
- The Monte-Carlo simulation shows that the risks associated with gasification are much lower according to the parameter variations presented in Tables 3-2 and 3-3. Therefore it is proven that gasification is a more mature technology and must be adopted for the future.

The economic analysis performed is both comprehensive and transparent allowing revision by readers wishing to use different economic assumptions. The results presented are conclusive and have a great deal of accuracy for the following reasons:

- Previous economic analyses performed on hydrogen production systems have always been focused on estimating the capital costs based on production capacities, operating pressure requirements and material of construction to determine a price of hydrogen in (\$/GJ). This study adopts a unique approach to confirm that SMR is in fact cheaper than gasification and is in agreement with published results. The uniqueness lies in the fact that a future selling hydrogen price was identified and cash flows were generated for both projects. This is a more economically sound method since it gives a clearer, more realistic idea of the investments with revenues generated at the end of each year.
- As opposed to the traditional method of using CPI to account for inflation, CEPCI was used. CEPCI was developed specifically to estimate costs of chemical engineering facilities. Since it is not influenced by other weighted factors, it results in greater accuracy.
- Most estimates developed used either the DDB or SL method of depreciation. This is not realistic and can create error in results. The MACRS approach used here represents the policy adopted by the I.R.S. to depreciate chemical facilities of this nature in a real-life situation.
- The cash flows developed are all discounted. While smaller projects can be evaluated by non-discounted cash flows they should not be used for such analyses. This ensures greater accuracy of results and follows a more realistic approach.

- A correlation was used to develop  $C_{OL}$ . While most estimates just assume the number of workers required and their hourly wages, a relation that differentiates between hours of operation of equipment and their operators, that accounts for shift-work for each process stage was used.
- And finally the Monte-Carlo simulation of probability distribution to quantify the associated risks was used to further strengthen results.
- The variation in  $C_{RM}$  has been modified to impart a more realistic approach based on previous cost data. This ensures greater accuracy of results from the Monte-Carlo simulation.

APPENDIX DATA FOR ECONOMIC ANALYSIS

Table A-1. Calculation of Fixed Capital Investment without Cost of Land ( $FCI_L$ ) for Steam Methane Reformation (SMR) and Gasification

| Method   | $FCI_L$<br>(million \$) |
|--|-------------------------|
| SMR<br>(includes natural gas preparation and handling, reformer, desulfurizer, heat recovery, shift converter, PSA and other related equipment, building, and facility)  | 136.1                   |
| Gasification<br>(includes coal storage, preparation and handling, air separation unit, gasifier, heat recovery/syngas cooling, shift converter, Sulfur removal and recovery systems, $CO_2$ absorption, removal and compression, PSA and other related equipment, building and facility) | 535.9                   |

Table A-2. Calculation of  $C_{RM}$  for Steam Methane Reformation (SMR) and Gasification

| Method       | Hydrogen production capacity (GJ) | Process efficiency (%) | Consumption of natural gas (GJ) | Price (\$/GJ) | $C_{RM}$ (million \$) |
|--------------|-----------------------------------|------------------------|---------------------------------|---------------|-----------------------|
| SMR          | 11,870,000                        | 85                     | 13,964,706                      | 7.50          | 105                   |
| Gasification | 11,870,000                        | 58                     | 20,465,517                      | 1.45          | 30                    |

Table A-3. Calculation of  $C_{UT}$  for Steam Methane Reformation (SMR) and Gasification

| Method   | Estimated consumption ( $10^6$ gallons) | Price (\$/1000 gallons) | $C_{UT}$ (million \$) |
|--|---|-------------------------|-----------------------|
| SMR<br>(water requirements for cooling and process steps)          | 4,000                                   | 0.5                     | 2.0                   |
| Gasification<br>(water requirements for cooling and process steps) | 12,000                                  | 0.5                     | 7.2                   |

Table A-4. Calculation of  $C_{OL}$  for Steam Methane Reformation (SMR) and Gasification

| Hydrogen production process | P | $N_{np}$ | $N_{OL}$ | $C_{OL}$ (million \$) |
|-----------------------------|---|----------|----------|-----------------------|
| SMR                         | 4 | 14       | 23       | 0.91                  |
| Gasification                | 6 | 16       | 34       | 1.36                  |

Table A-5. Calculation of Economic Analysis Parameters for Steam Methane Reformation (SMR) and Gasification

| Economic parameters  | SMR           | Gasification  |
|--|---------------|---------------|
| Taxation rate  | 42 %          | 42 %          |
| Annual interest rate   | 10 %          | 10 %          |
| Salvage value  | \$13,610,000  | \$53,590,000  |
| Working capital  | \$24,201,000  | \$56,726,000  |
| FCI <sub>L</sub>   | \$136,100,000 | \$535,900,000 |
| Revenue from sales   | \$249,270,000 | \$249,270,000 |
| Cost of raw materials, C <sub>RM</sub>                       | \$105,000,000 | \$30,000,000  |
| Cost of utilities, C <sub>UT</sub>                           | \$2,410,000   | \$7,234,000   |
| Cost of operating labor, C <sub>OL</sub>                     | \$910,000     | \$1,360,000   |
| Cost of manufacturing without depreciation, COM <sub>d</sub> | \$159,096,600 | \$149,972,620 |
| Project life (years after startup)                           | 20            | 20            |
| Construction period  | 3             | 3             |
| Distribution of FCI <sub>L</sub>                             |               |               |
| End of year one  | 10 %          | 10 %          |
| End of year two  | 35 %          | 35 %          |
| End of year three  | 55 %          | 55 %          |

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