HYDROGASIFICATION OF COAL FOR HYDROGEN PRODUCTION WITH REDUCED CO₂ EMISSION

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ABSTRACT:

A hydrogasification process is presented to produce hydrogen from coal, which is more efficient than the conventional steam / oxygen gasification process and with lower CO₂ emissions. Hydrogasification of coal is an exothermic process whereas steam gasification is an endothermic process, which requires oxygen. A technical and economic comparison is made for three processes, which includes the catalytic steam gasification of coal. Hydrogasification has been found to be the most economical.

Although the hydrogasification process can be practiced above ground with mined coal, the process can be performed with unmined coal in a process termed Pumped Carbon Mining (PCM). PCM is especially advantageous for unminable seams; such as in depleted coal bedded methane (CBM) wells. PCM opens a new resource for generating hydrogen in an economically attractive manner.

KEYWORDS : hydrogen, coal, hydrogasification.

Introduction

Because of the availability and low price stability of coal in the United States compared to limited resource and high cost of natural gas and oil in the U.S., it becomes increasingly apparent that coal will become the prime feedstock for production of hydrogen in the U.S. in support of the so called hydrogen economy in the future. The conventional current industrial process for the production of hydrogen in the U.S. is the steam reforming of natural gas. The conventional process for hydrogen production from coal is the steam – oxygen gasification of coal. A catalytic steam gasification of coal process has also been presented. A hydrogasification process of coal is proposed which holds out the promise of being more efficient and more economical than the conventional process for production of hydrogen from coal. In the following, a description and comparison is made for each of these processes. The comparison is made with a N. Dakota lignite coal feedstock with the composition and physical and thermodynamic properties given in table 1 among other feedstocks.

1. Steam – Oxygen Gasification

Table 2 shows the process chemistry unit operations and mass and energy balances for the lignite steam–oxygen gasification process. Fig. 1 gives a process flow sheet for hydrogen production. A main feature of this process is that the gasification reaction is endothermic. The reaction is usually conducted at about 900°C and 50 atm pressure. Various gasifier reactors have been used to conduct the gasification including Texaco Entrained Flow Reactor, Lurgi Slagging Gasifier and Koppers Totzek High Temperature Gasifier. One of the largest array of Lurgi gasifiers is located in the SNG (Substituted Natural Gas) Dakota Gasification Co. plant in Beulah North Dakota. In order to provide the endothermic energy for the steam gasification, an oxygen plant supplies oxygen to the gasifier so that part of the coal fed is burned in the reactor. The elimination of nitrogen from the air is of importance in coal gasification plants so that the
synthesis gas (H₂ and CO) produced does not become diluted. Due to equilibrium and heat losses in the reactor, as much as double the coal is required to make up for the energy balance of the endothermic reaction. It is also important to add sufficient steam to the gasifier to form the CO and H₂ synthesis gas. The H₂ and CO synthesis gas effluent together with equilibrium quantities of H₂O and CO₂ is sent to a hot gas cleanup, which removes the contaminants H₂S, NH₃ and particulates. Adsorbents and reactants, such as zinc oxide, are used in the hot gas cleanup. After cooling down the gases in a heat exchanger to about 250°C, the gas is sent to a water gas shift where the CO is reacted with steam to form hydrogen and carbon dioxide. Finally, the CO₂ is separated either by pressure swing adsorption (PSA) or cryogenically, producing the hydrogen product gas. The CO₂ emitted is of high concentration, which can be either sequestered avoiding greenhouse gas emissions or sold, especially for the expanding market of Enhanced Oil Recovery (EOR). At the bottom of Table 2, the thermal efficiency of conversion of lignite to hydrogen energy (HHV) is calculated to be 63.2%. This does not take into account the energy in steam that can be used as process heat for other purposes.

An estimate of the capital investment for a larger (>100 million- SCF H₂ / D) coal (lignite) based hydrogen plant can be determined from an updated investment in the North Dakota Plant, and eliminating the methanator reactor. The capital investment results in a value of $5,360 / MMBTU / Day or $1,729 / MSCF H₂ / D. Lignite cost is now about $1 / MMBTU in Montana. A total fixed charge rate of 20% on investment is assumed, which includes a 20 year plant life depreciation, 10% return on investment and tax rate of 50% of net profit. Operation and maintenance is assumed to be 15% of fixed charges. An 80% plant factor is assumed.

### HYDROGEN PRODUCTION COST FOR STEAM–OXYGEN COAL GASIFICATION PLANT

<table>
<thead>
<tr>
<th></th>
<th>$/ MMBTU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lignite $1.00 / 0.632</td>
<td>1.58</td>
</tr>
<tr>
<td>Fixed Charges (0.20 x $5,360/0.8x365)</td>
<td>3.67</td>
</tr>
<tr>
<td>Op and Maint. (0.15 x 3.67)</td>
<td>0.55</td>
</tr>
<tr>
<td>Production Cost</td>
<td>$5.80/ MMBTU</td>
</tr>
<tr>
<td></td>
<td>$1.87 / MSCF</td>
</tr>
<tr>
<td></td>
<td>$0.70 / gal gasoline equivalent (gge)</td>
</tr>
</tbody>
</table>

**2) Catalytic Steam Gasification**

Table 3 gives the process chemistry and energy balance for the catalytic steam gasification of lignite and Fig. 2 shows the flow sheet for the process. The process was originally developed by Exxon in the 1970’s. The purpose of the catalyst is to reduce the temperature in the gasifier so as to direct the reaction towards producing methane and reducing H₂ and CO synthesis gas. This makes the process much less endothermic and allows the elimination of an oxygen plant. The catalytic gasifier reaction is slightly endothermic; the energy being provided by the heat input of the steam recycled from the methane reformer. After hot gas cleanup, the methane is steam reformed to produce additional hydrogen. The gasifier catalyst consists of potassium carbonate mixed in large quantities of about 20% by weight of the coal feed. In order to maintain concentrations below thermodynamic equilibrium H₂ and CO are recycled to the catalytic gasifier. The steam reformer converts the methane to hydrogen and CO. The CO is converted to hydrogen and CO₂ in a water gas shift reactor. The CO₂ is separated from the hydrogen gas to produce pure hydrogen product stream. Equivalent hydrogen energy is required to provide the slight endothermic energy in the gasifier and to process the recovery of catalyst from the ash. The net thermal efficiency for this process is 71.5% conversion of the energy in the lignite to hydrogen energy. This efficiency is 13% higher than the steam-oxygen gasification. An estimate of the production cost assumes the capital investment is about the same as the steam-oxygen gasification plant $5,360 / MMBTU / Day, $1,729 / MSCF H₂ / D. The catalyst cost assumes that 1% of the weight of the coal carrying 20% catalyst is lost and has to be replaced at a cost of $500 / ton K₂CO₃.
HYDROGEN PRODUCTION COST FOR CATALYTIC STEAM COAL GASIFICATION PLANT

<table>
<thead>
<tr>
<th></th>
<th>$/ MMBTU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lignite $1.00 / 0.715</td>
<td>1.39</td>
</tr>
<tr>
<td>Fixed Charges (0.20 x $5.360/0.8x365)</td>
<td>3.67</td>
</tr>
<tr>
<td>Op and Maint. (0.15 x 3.67)</td>
<td>0.55</td>
</tr>
<tr>
<td>Catalyst Cost</td>
<td>0.41</td>
</tr>
<tr>
<td>Production Cost</td>
<td>$6.02/ MMBTU</td>
</tr>
<tr>
<td></td>
<td>$1.94 / MSCF</td>
</tr>
<tr>
<td></td>
<td>$0.72 / gal gasoline equivalent</td>
</tr>
</tbody>
</table>

Because of the catalyst cost, the hydrogen production cost is slightly higher than the steam-oxygen gasification process.

3) Hydrogasification of Mined Coal Above Ground

Fig. 3 shows the process flow sheet and Table 4 gives the process chemistry and energy balance of the hydrogasification of mined lignite to produce hydrogen. There exists much laboratory data on coal hydrogasification. A 10 tons / hr pilot plant has been constructed and operated in Germany in the early 1980’s. A main feature of this process is that the hydrogasification reaction is exothermic, which makes the process more thermally energy efficient and does not require an oxygen plant. The concentration of methane produced in the hydrogasification is equilibrium limited so that practically about 40% by volume methane at temperature of about 850°C and a pressure of about 70 atm is attainable. This means that a large circulating load of hydrogen gas must be maintained through the process. There is no need to separate the methane for steam reforming to produce additional H₂ and CO. The temperature of hydrogasification can be controlled by injection of a small amount of oxygen into the hydrogen, which forms steam and quenches the exothermic reaction. A water gas shift follows the steam reformer. The CO₂ is removed by Pressure Swing Adsorption (PSA) or cryogenically and is ready for marketing or sequestration without further processing. The steam reformer is heated by combustion of part of the hydrogen so there is no emission of CO₂ from the reformer. The thermal efficiency of this process is calculated to be 73.2%, which is 16% higher than the steam-oxygen gasification plant. The CO₂ emission is also 16% lower than the steam-oxygen gasification.

Because a costly air separation plant is eliminated from the process as well as a catalyst-processing step with the addition of a not so costly steam-reforming step, the capital investment for hydrogasification becomes lower than either of the two previous processes. It is therefore estimated that the capital investment will be about 80% of the steam-oxygen and catalytic gasification.

The capital investment for the hydrogasification process is then $4,288 / MMBTU or $1,383 / MSCF H₂. A large part of the capital investment is attributed to the steam reforming plant. Newer plants are estimated to have even lower unit investment cost than assessed in this paper.

HYDROGEN PRODUCTION COST FOR MINED COAL HYDROGASIFICATION PLANT

<table>
<thead>
<tr>
<th></th>
<th>$/ MMBTU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lignite $1.00 / 0.732</td>
<td>1.37</td>
</tr>
<tr>
<td>Fixed Charges (0.20 x $4,288/0.8x365)</td>
<td>2.94</td>
</tr>
<tr>
<td>Op and Maint. (0.15 x 2.94)</td>
<td>0.44</td>
</tr>
<tr>
<td>Production Cost</td>
<td>$4.75/ MMBTU</td>
</tr>
<tr>
<td></td>
<td>$1.53 / MSCF</td>
</tr>
<tr>
<td></td>
<td>$0.57 / gal gasoline equivalent</td>
</tr>
</tbody>
</table>

Thus, hydrogasification production cost is 18% lower than the steam-oxygen plant.

4) Underground Hydrogasification of Coal (Pumped Carbon Mining, PCM)

The in situ underground hydrogasification of coal for hydrogen production is similar to the above ground process with the exception that the hydrogasification reaction takes place underground. Although the process can be applied in any coal mine, it is especially useful for unminable seams and where methane is produced from coal bedded methane operations (CBM) in depleted wells.
In one configuration, the coal seam is accessed by two vertical boreholes spaced a distance apart: one is an injection borehole and the other is an extraction borehole. A flow connection is established between the boreholes by horizontal directional drilling or by a burn-back\(^{(1)}\) technique. During the CBM process, the water that may exist between the linked boreholes is removed, which is beneficial to the subsequent hydrogasification process. A schematic of the system is shown in Fig. 4 including the above ground processing.

Heated and pressurized hydrogen is injected into the seam, which reacts with the coal producing methane and carbon monoxide and releases heat due to the exothermicity of the reaction. To initiate the process, some hydrogen supply will be used to burn with air to preheat the hydrogen to reaction temperatures. Once the exothermic reaction is established, the process is self-sustaining and the temperature is controlled by the injection of oxygen, which forms steam and quenches the reaction. The process chemistry and energy balance is shown in Table 4, described previously for the above ground mined coal process.

An excess of hydrogen is used to convert the coal, which is limited by thermodynamic equilibrium at temperatures between about 800 and 900\(^{\circ}\)C and pressures between about 50 and 100 atm. The recovered gas from the extraction borehole is subject to hot gas cleanup, where the H\(_2\)S and NH\(_3\) and particulates are removed, leaving a methane rich streams (40% by vol.) and carbon monoxide in an excess of hydrogen. The cleaned gas is then sent to a steam reformer, which converts the methane to CO and H\(_2\). The endothermic heat required in the reformer is provided by indirect heating of the reformer tubes containing catalyst using hydrogen burners. In this manner, no CO\(_2\) is emitted in the process. The reformed gas is heat exchanged with cooler recirculating hydrogen to about 250\(^{\circ}\)C and sent to a water gas shift reactor where the CO is converted with steam to CO\(_2\) and H\(_2\). Finally, the CO\(_2\) is removed by PSA or cryogenically. The effluent hydrogen is directed into 3 streams, one for production, one for use as a fuel in the steam reformer and the third for circulating and for hydrogasifying the underground coal seam. The thermal efficiency of conversion of lignite to hydrogen is the same as the above ground process, which is indicated in Table 4 as 73.2% and assumes a 90% utilization of the coal.

It should be noted that the catalytic process is not applicable for underground processing of coal because it is not practical to inject large quantities of K\(_2\)CO\(_3\) catalyst underground, which would not be recoverable.

5) Hydrogen Production Cost for Underground Hydrogasification of Unmined Coal
When applying underground hydrogasification to depleted coal bedded methane operations, the cost of underground site preparation (borehole and horizontal drilling) is borne by the CBM operation so that the investment is only in above ground processing equipment. The underground operation eliminates the above ground coal hydrogasifier and reduces the capital investment by 25% compared to above ground hydrogasification. This results in a unit capital investment of $3,216 / MMBTU / Day or $1,036 / MSCF /Day. Furthermore, the cost of mining the lignite coal is eliminated.

<table>
<thead>
<tr>
<th>HYDROGEN PRODUCTION COST FOR PUMPED CARBON MINING HYDROGASIFICATION PLANT</th>
<th>$/ MMBTU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed Charges (0.20 x $3,216/0.8x365)</td>
<td>2.20</td>
</tr>
<tr>
<td>Op and Maint. (0.15 x 2.30)</td>
<td>0.33</td>
</tr>
<tr>
<td>Production Cost</td>
<td>$2.53 / MMBTU</td>
</tr>
<tr>
<td></td>
<td>$0.81 / MSCF</td>
</tr>
<tr>
<td></td>
<td>$0.30 / gal gasoline equivalent</td>
</tr>
</tbody>
</table>

Because a single CBM well usually yields less than 500 MSCF / D of CBM (CH\(_4\))\(^{(6)}\) the coal in the seam could increase the methane production capacity 20-fold to 10,000 MSCF / D of methane. Since 2.8 MSCF (H\(_2\)) / MSCF (CH\(_4\)) is produced, it would take at least 4 wells to bring the total hydrogen production capacity to above 100,000 MSCF, which is the equivalent capacity of a modern steam reforming plant. Thus, one central hydrogasification facility must service a number of CBM wells by collection, storage and conversion of methane produced from the coal to hydrogen.

6) Conclusion
A summary comparison of the three processes investigated in this paper is given in Table 5. The hydrogasification process appears to be the more economical being 16% more efficient and 18% more economical than the conventional steam-oxygen process. The CO\(_2\) emission is also 15% less than the steam-oxygen plant, which is the hydrogasification application to an underground depleted CBM well that gives the greatest reduction in hydrogen production cost, namely 57% lower than the above ground. Although a steam-oxygen process can be practiced underground, based on the above ground estimates in
this paper, hydrogasification underground is still more economical. A similar study for above and below ground processes for conversion of coal to substitute natural gas (SNG) indicates the same conclusion. At current $10 / MSCF cost of natural gas, the cost of hydrogen production by conventional steam reforming is of the order of one $4 / MSCF H₂ ($1.50 / gge), natural gas making up 80% of the production cost. The incentive for conducting hydrogasification of coal, especially underground production of hydrogen at $0.84 / MSCF ($0.30 / gge), is compelling. A limited field test for underground coal hydrogasification at a depleted CBM site to prove out the system is greatly justified.

### Table 1

**Basic Data for Coal and Biomass Feedstocks Used in the Study**  
**Composition and Thermodynamic Data**

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Biomass Wood</th>
<th>Bituminous Kentucky Coal</th>
<th>Lignite N. Dakota Coal</th>
<th>Sub-bituminous Wyodak Coal</th>
<th>Alaskan Beluga Coal</th>
<th>Sewage Sludge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition (wt%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>45.86</td>
<td>67.02</td>
<td>43.37</td>
<td>49.95</td>
<td>49.33</td>
<td>28.55</td>
</tr>
<tr>
<td>H</td>
<td>5.27</td>
<td>4.54</td>
<td>2.78</td>
<td>3.51</td>
<td>4.00</td>
<td>4.09</td>
</tr>
<tr>
<td>O</td>
<td>36.07</td>
<td>7.22</td>
<td>13.97</td>
<td>12.58</td>
<td>15.56</td>
<td>6.03</td>
</tr>
<tr>
<td>H₂O</td>
<td>11.67</td>
<td>8.60</td>
<td>30.10</td>
<td>26.40</td>
<td>21.78</td>
<td>9.82</td>
</tr>
<tr>
<td>Ash</td>
<td>0.04</td>
<td>2.85</td>
<td>0.81</td>
<td>0.60</td>
<td>0.12</td>
<td>1.36</td>
</tr>
<tr>
<td>N</td>
<td>0.43</td>
<td>1.43</td>
<td>0.67</td>
<td>0.93</td>
<td>0.54</td>
<td>3.62</td>
</tr>
<tr>
<td>Molar Composition (MAF)</td>
<td>CH₁.₃₃O₀.₅₉</td>
<td>CH₀.₈₁O₀.₀₈</td>
<td>CH₀.₇₇O₀.₂₄</td>
<td>CH₀.₈₄O₀.₁₉</td>
<td>CH₀.₉₇O₀.₂₄</td>
<td>CH₁.₇₂O₀.₄₂</td>
</tr>
<tr>
<td>MW</td>
<td>22.82</td>
<td>14.09</td>
<td>16.61</td>
<td>15.88</td>
<td>16.81</td>
<td>20.44</td>
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<tr>
<td>Heating Value (HHV)</td>
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<td></td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>BTU/lb MF</td>
<td>-8800.0</td>
<td>-13650</td>
<td>-10254</td>
<td>-11730</td>
<td>-11082</td>
<td>-5510</td>
</tr>
<tr>
<td>kcal/kg MF</td>
<td>-4888.9</td>
<td>-7583.3</td>
<td>-5696.7</td>
<td>-6516.7</td>
<td>-6156.7</td>
<td>-3061.1</td>
</tr>
<tr>
<td>kcal / g-mol MAF</td>
<td>-112.8</td>
<td>-119.0</td>
<td>-110.3</td>
<td>-115.3</td>
<td>-117.5</td>
<td>-115.9</td>
</tr>
<tr>
<td>Heat of Formation (MAF)</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>kcal/kg</td>
<td>-1214.4</td>
<td>-183.0</td>
<td>-593.0</td>
<td>-461.7</td>
<td>-584.9</td>
<td>-1769.7</td>
</tr>
<tr>
<td>ΔH_f kcal/g-mol</td>
<td>-27.7</td>
<td>-2.6</td>
<td>-9.8</td>
<td>-7.3</td>
<td>-9.8</td>
<td>-36.2</td>
</tr>
<tr>
<td>Heat Capacity (kcal/Kg MF / °C)</td>
<td>0.570</td>
<td>0.315</td>
<td>0.315</td>
<td>0.315</td>
<td>0.315</td>
<td>0.250</td>
</tr>
<tr>
<td>kcal/kg MF/°C</td>
<td>13.00</td>
<td>4.44</td>
<td>5.23</td>
<td>5.00</td>
<td>5.30</td>
<td>5.11</td>
</tr>
<tr>
<td>Moisture</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Mol H₂O / mol C</td>
<td>0.170</td>
<td>0.086</td>
<td>0.462</td>
<td>0.353</td>
<td>0.294</td>
<td>0.230</td>
</tr>
</tbody>
</table>

*From various sources, thermodynamic tables and calculated values.
Table 2
Steam-Oxygen Coal Gasification for Hydrogen Production
Unit Operation and Process Chemistry
Coal Feedstock – Lignite – Basis 1 g-mol

1. Steam-Oxygen Gasification of Lignite

REACTION CHEMISTRY

(1) Coal Gasifier - Lignite Coal Feed

\[
\text{CH}_{0.8} \text{O}_{0.2} + 0.8 \text{ H}_2\text{O} = 1.2 \text{ H}_2 + \text{CO}
\]

\[\Delta H = + 38.2 \text{ Kcal / g-mol lignite} – \text{endothermic – 90% lignite conversion}\]

Energy Provided by Lignite Combustion with Oxygen Feed

\[
\text{CH}_{0.8} \text{O}_{0.2} + 1.1 \text{ O}_2 = 0.4 \text{ H}_2\text{O} + \text{CO}_2
\]

\[\Delta H = - 110.3 \text{ Kcal / g-mol} – \text{exothermic}\]

Lignite Required \(= \frac{38.2}{110.3} = 0.35 \text{ g-mol}\)

Due to Equilibrium, Heat Loss and Inefficiency of the Gasifier, this Increases to 0.70 g-mol at 50% eff.

(2) Air separation plant for oxygen production: An electricity powered cryogenic process.

Equivalent Coal Power Plant Energy Required \(= 25.4 \text{ Kcal / g-mol Lignite (at 300 Kwh(e) / ton O}_2\)

(3) Hot Gas Cleanup removes N, S & particulates

(4) Water Gas Shift for H\(_2\) Production

\[
\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2
\]

\[\Delta H = 0.0 \text{ Kcal / g-mol CO}\]

(5) Gas Separator, e.g. Differential Pressure Swing Adsorption (PSA) or Cryogenic Separation, removes CO\(_2\) and produces H\(_2\)

(6) Overall Reaction

\[
\text{CH}_{0.8} \text{O}_{0.2} + 1.8 \text{ H}_2\text{O} = 2.2 \text{ H}_2 + \text{CO}_2
\]

\[
\text{HHV Thermal Efficiency} = \frac{2.2 \times 68.0 \times 0.9}{(1.0 + 0.70)110.3 + 25.4} \times 100 = 63.2\%
\]

Net production \(= 1.03 \text{ g-mol H}_2 / \text{ g-mol lignite}\)
Table 3
Catalytic Steam Gasification of Coal for Hydrogen Production
Unit Operation and Process Chemistry
Coal Feedstock – Lignite – Basis 1 g-mol

(1) Catalytic Steam Gasification of Lignite at 700°C and 35 ATM
\[ CH_{0.8}O_{0.2} + 0.7 \text{ H}_2\text{O} = 0.55 \text{ CH}_4 + 0.45 \text{ CO}_2 \]
\[ \Delta H = + 5.2 \text{ Kcal / g-mol lignite} \] – endothermic – 90% lignite conversion
This Energy Is Provided In Steam Reformer at 80% efficiency = +6.5 Kcal / g-mol
Takes 6.5/68 = 0.1 g-mol H\(_2\) combustion energy
In Presence of K\(_2\)CO\(_3\) Catalyst
Catalyst Content is 20% of Lignite Feed By Weight
Coal Conversion Efficiency = 90%

(2) Separation and Recovery of K\(_2\)CO\(_3\) from Ash Containing Silica and Alumina
Takes 0.20 g-mol H\(_2\) of Equivalent Energy for Process per g-mol Lignite
\[ \Delta H = + 13.6 \text{ Kcal} \]

(3) Steam Reforming the Methane at 800°C and 70 ATM
\[ 0.55 \text{ CH}_4 + 0.55 \text{ H}_2\text{O} = 0.55 \text{ CO} + 1.65 \text{ H}_2 \]
\[ \Delta H = - 33.0 \text{ Kcal / g-mol} \] – endothermic
Hydrogen Combustion Provides the Energy: \( H_2 + \frac{1}{2} \text{ O}_2 = \text{ H}_2\text{O}\)
\[ \Delta H = - 68 \text{ Kcal / g-mol} \] at 80% eff: \( H_2 = \frac{33}{0.8} \times 68 = 0.61 \text{ g-mol} \)

(4) Water Gas Shift
\[ 0.55 \text{ CO} + 0.55 \text{ H}_2\text{O} = 0.55 \text{ CO}_2 + 0.55 \text{ H}_2 \] \( \Delta H = 0.0 \)

(5) Gas Separator, e.g. Differential Pressure Swing Adsorption or Cryogenic Separation
Separates H\(_2\) from CO\(_2\)
Overall Reaction: \( CH_{0.8}O_{0.2} + 1.8 \text{ H}_2\text{O} = 2.2 \text{ H}_2 + 1.0 \text{ CO}_2 \)
Net hydrogen produced = \([1.65 + 0.55 - (0.61 + 0.20 + 0.10)] \times 0.9 \]
\[ 1.16 \text{ g-mol H}_2 / \text{ g-mol lignite} \]
Thermal Efficiency = \([0.9 \times 1.29 \times 68]/110.3 \] \times 100 = 71.5%

Table 4
Coal Hydrogasification for Hydrogen Production
Unit Operation and Process Chemistry
Coal Feedstock – Lignite – Basis 1 g-mol

(1) Hydrogasification of Lignite
\[ CH_{0.8}O_{0.2} + 1.2 \text{ H}_2 = 0.8 \text{ CH}_4 + 0.2 \text{ CO} \]
\[ \Delta H = -9.8 \text{ Kcal / g-mol lignite} \] – exothermic 90% lignite conversion

(2) Hot Gas Cleanup removes N, S & particulates

(3) Steam Reforming of Methane
\[ 0.8 \text{ CH}_4 + 0.8 \text{ H}_2\text{O} = 0.8 \text{ CO} + 2.4 \text{ H}_2 \]
\[ \Delta H = + 48.0 \text{ Kcal / g-mol} \] – endothermic
Hydrogen Combustion Provides the Energy at 80% efficiency = 48/68 x 0.8 = 0.88 g-mol H\(_2\)

(4) Water Gas Shift of all the CO
\[ 1.0 \text{ CO} + 1.0 \text{ H}_2\text{O} = 1.0 \text{ CO}_2 + 1.0 \text{ H}_2 \]
\[ \Delta H = 0.0 \]

(5) Overall Stoichiometric Reaction
\[ CH_{0.8}O_{0.2} + 1.8 \text{ H}_2\text{O} = 2.2 \text{ H}_2 + 1.0 \text{ CO}_2 \]

(6) Net Production of H\(_2\) = \((2.20 - 0.88) \times 0.9 = 1.19 \text{ g-mol} / \text{ g-mol lignite} \)

(7) Overall Thermal Efficiency of the Coal to Hydrogen Energy
\[ = \frac{(0.9 \times 1.32 \times 68)/110.3}{100} = 73.2% \]
<table>
<thead>
<tr>
<th>Process</th>
<th>Steam-Oxygen Gasification</th>
<th>Catalytic Steam Gasification</th>
<th>Hydrogasification</th>
<th>Underground Gasification Pumped Carbon Mining (PCM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Feedstock (Lignite)</td>
<td>Mined – Crushed – Transported</td>
<td>Mined – Crushed – Transported</td>
<td>Mined – Crushed – Transported</td>
<td>Depleted Unminable Coal Seam</td>
</tr>
<tr>
<td>Oxygen Plant</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
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<tr>
<td>Gasifier Type</td>
<td>Steam – Oxygen</td>
<td>Steam</td>
<td>Hydrogen</td>
<td>Hydrogen</td>
</tr>
<tr>
<td>Steam Methane Reformer</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Thermal Efficiency Coal to Hydrogen</td>
<td>63.2</td>
<td>71.5</td>
<td>73.2</td>
<td>73.2</td>
</tr>
<tr>
<td>CO₂ Emission</td>
<td>102</td>
<td>90</td>
<td>87</td>
<td>87</td>
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<tr>
<td>Lbs CO₂ / MSCF H₂</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>% Increase in efficiency from Steam-Oxygen</td>
<td>0</td>
<td>13</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>Capital Investment $ / MSCF H₂ / day</td>
<td>1729</td>
<td>1729</td>
<td>1383</td>
<td>1036</td>
</tr>
<tr>
<td>Production Cost $ / MSCF H₂</td>
<td>1.87</td>
<td>1.94</td>
<td>1.53</td>
<td>0.81</td>
</tr>
<tr>
<td>% Cost reduction from Steam-Oxygen</td>
<td>0</td>
<td>4% Increase</td>
<td>18</td>
<td>57</td>
</tr>
</tbody>
</table>
**FIG 1. STEAM-OXYGEN COAL GASIFICATION FOR HYDROGEN PRODUCTION**

**REACTION CHEMISTRY**

1. Coal Gasifier - Lignite Coal Feed
   \[ CH_3O \cdot O_2 + 0.8 \cdot H_2O = 1.2 \cdot H_2 + CO_2 \quad \text{Delta H} = +38.2 \text{ Kcal/g-mol lignite - endothermic} \]
   Lignite Combustion
   \[ CH_3O \cdot O_2 + 1.1 \cdot O_2 = 0.4 \cdot H_2O + CO_2 \quad \text{Delta H} = -110.3 \text{ Kcal/g-mol - exothermic} \]
   at 50% efficiency 0.7 g-mol lignite/lignite feed required

2. Hot Gas Cleanup removes N, S & particulates

3. Water Gas Shift CO + H_2O = CO_2 + H_2 \quad \text{Delta H} = 0.0 \text{ Kcal/g-mol CO}

4. Gas Separator, e.g. Differential Pressure Swing Adsorption or Cryogenic Separation, separates H_2 and CO_2

5. Overall Reaction \[ CH_3O \cdot O_2 + 1.8 \cdot H_2O = 2.2 \cdot H_2 + CO_2 \]

6. Net production = 1.03 g-mol H_2 / g-mol lignite (90% lignite conversion)

**FIG 2. CATALYTIC GASIFICATION OF COAL FOR HYDROGEN PRODUCTION**

**REACTION CHEMISTRY**

1. Catalytic Gasifier - Lignite Coal Feed
   \[ CH_3O \cdot O_2 + 0.7 \cdot H_2O = 0.55 \cdot CH_4 + 0.45 \cdot CO_2 \quad \text{Delta H} = +5.2 \text{ Kcal/g-mol lignite - endothermic} \]

2. Hot Gas Cleanup removes N, S & particulates

3. K_2CO_3 / Ash Separation = Equivalent H_2 Energy Required Delta H = +33.6 Kcal

4. Steam Reforming the Methane
   \[ 0.55 \cdot CH_4 + 0.55 \cdot H_2O = 0.55 \cdot CO + 1.65 \cdot H_2 \quad \text{Delta H} = -33.0 \text{ Kcal/g-mol - endothermic} \]

5. Water Gas Shift 0.55 CO + 0.55 H_2O = 0.55 CO_2 + 0.55 H_2

6. Gas Separator, e.g. Differential Pressure Swing Adsorption or Cryogenic Separation, separates H_2 and CO_2

7. Overall reaction 1.16 CH_3O \cdot O_2 + 1.8 H_2O = 2.2 H_2 + 1.0 CO_2

8. Net production = 1.16 g-mol H_2 / g-mol lignite (at 90% lignite conversion)
**FIG 3. COAL HYDROGASIFICATION FOR HYDROGEN PRODUCTION**

**REACTION CHEMISTRY**

1. Hydrogasifier - Lignite Coal Feed
   
   \[ \text{CH}_4 + \text{O}_2 + 1.2 \; \text{H}_2 = 0.8 \; \text{CH}_4 + 0.2 \; \text{CO} \quad \text{Delta H} = -9.8 \text{ Kcal/g-mol lignite - exothermic} \]

2. Hot Gas Cleanup removes N, S & particulates

3. Steam Reforming the Methane
   
   \[ 0.8 \; \text{CH}_4 + 0.8 \; \text{H}_2 = 0.8 \; \text{CO} + 2.4 \; \text{H}_2 \; \text{O} \quad \text{Delta H} = +48.0 \text{ Kcal/g-mol - endothermic} \]
   
   \[ 0.88 \; \text{g-mol} \; \text{H}_2 \; \text{burned with air} \; \text{Delta H} = +48.0 \text{ Kcal/g-mol} \]

4. Water Gas Shift
   
   \[ 1.0 \; \text{CO} + 1.0 \; \text{H}_2 \; \text{O} = 1.0 \; \text{CO}_2 + 1.0 \; \text{H}_2 \quad \text{Delta H} = 0.0 \text{ Kcal/g-mol CO} \]

5. Overall Reaction
   
   \[ \text{CH}_4 + \text{O}_2 + 1.8 \; \text{H}_2 \; \text{O} = 1.0 \; \text{CO}_2 + 2.2 \; \text{H}_2 \]

6. Net production = 1.19 g-mol H2/g-mol lignite (at 90% lignite conversion)

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**FIG 4. UNDERGROUND COAL HYDROGASIFICATION (PUMPED CARBON MINING) HYDROGEN PRODUCTION**

**REACTION CHEMISTRY**

1. Hydrogasifier - Lignite Coal Feed
   
   \[ \text{CH}_4 + \text{O}_2 + 1.2 \; \text{H}_2 = 0.8 \; \text{CH}_4 + 0.2 \; \text{CO} \quad \text{Delta H} = -9.8 \text{ Kcal/g-mol lignite - exothermic} \]

2. Hot Gas Cleanup removes N, S & particulates

3. Steam Reforming the Methane
   
   \[ 0.8 \; \text{CH}_4 + 0.8 \; \text{H}_2 = 0.8 \; \text{CO} + 2.4 \; \text{H}_2 \; \text{O} \quad \text{Delta H} = +48.0 \text{ Kcal/g-mol - endothermic} \]
   
   \[ 0.88 \; \text{g-mol} \; \text{H}_2 \; \text{burned with air} \; \text{Delta H} = +48.0 \text{ Kcal/g-mol} \]

4. Water Gas Shift
   
   \[ 1.0 \; \text{CO} + 1.0 \; \text{H}_2 \; \text{O} = 1.0 \; \text{CO}_2 + 1.0 \; \text{H}_2 \quad \text{Delta H} = 0.0 \text{ Kcal/g-mol CO} \]

5. Overall Reaction
   
   \[ \text{CH}_4 + \text{O}_2 + 1.8 \; \text{H}_2 \; \text{O} = 1.0 \; \text{CO}_2 + 2.2 \; \text{H}_2 \]

6. Net production = 1.19 g-mol H2/g-mol lignite (at 90% lignite conversion)
References:
6) M. Steinberg, “Pumped Carbon Mining (PCM) for Substitute Natural Gas Production,” Report HCEI-10-04-3r1, HCE, LLC, Oakton, VA (October 3, 2004).
8) M. Gatens, Oil and Gas J., 41-3 (December 13, 2004).