



NATIONAL ENERGY TECHNOLOGY LABORATORY



# Evaluation of Alternate Water Gas Shift Configurations for IGCC Systems

August 5, 2009

DOE/NETL-401/080509



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# **Evaluation of Alternate Water Gas Shift Configurations for IGCC Systems**

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# **1 Executive Summary**

As carbon control in Integrated Gasification Combined Cycle (IGCC) systems gains increasing awareness, emphasis is placed on optimization of the water-gas shift (WGS) reaction. This process step is required to convert carbon to a form ( $\text{CO}_2$ ) that can be separated from coal-derived syngas by a conventional acid gas removal system. The extent to which CO is converted to  $\text{CO}_2$  is determined by the degree of carbon capture required. This analysis considers a range of carbon capture goals (60-90%) and evaluates several WGS configurations and steam consumption scenarios that could potentially accommodate each capture target, while realizing cost and efficiency benefits.

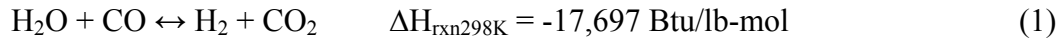
In order to drive the reaction equilibrium toward the water gas shift products ( $\text{H}_2$  and  $\text{CO}_2$ ), steam is typically introduced at the inlet of the shift reactor. This shift steam is taken from an intermediate extraction point in the steam turbine. Any steam extracted for the shift is not expanded in the turbine to produce power, therefore the water gas shift step is typically viewed as a burden on the steam cycle.

This analysis considers the technical and economic implications of reductions in shift steam consumption. This reduction will improve steam cycle performance (and system efficiency) by allowing for the expansion of a greater mass of steam through the turbine. However it will also result in larger water gas shift reactors to achieve the same level of CO conversion, increasing capital costs. The tradeoff between improved efficiency and higher capital cost is the focus of this study.

This study finds that although capital costs increase due to larger reactor volume, the savings in shift steam is more than adequate to offset this loss. For all cases considered (with the exception of 90% carbon capture), a shift steam reduction resulted in cost and efficiency improvements. However 90% carbon capture is only possible by feeding high levels of shift steam, to drive the reaction equilibrium toward the products. A lower limit does exist with respect to the minimum amount of shift steam required. If shift steam levels are too low, the required reactor volume becomes prohibitively large, therefore negating the benefit of steam savings.

## 2 Background

As carbon control in IGCC systems gains increasing awareness, emphasis is placed on optimization of the water gas shift (WGS) reaction. The WGS reaction converts CO to CO<sub>2</sub>, consuming one mole of steam and producing one mole of hydrogen in the process:



This process step is required to convert carbon to a form (CO<sub>2</sub>) that can be separated from coal-derived syngas by a conventional acid gas removal system. The extent to which CO is converted to CO<sub>2</sub> is determined by the degree of carbon capture required. This analysis considers a range (60-90%) of carbon capture<sup>i</sup> goals and evaluates several WGS configurations and steam-to-dry gas (S:DG) molar ratios that could potentially accommodate each capture target, while realizing cost and efficiency benefits. The study was inspired by a presentation at the 2006 Gasification Technologies Council Annual Meeting by Rao, Verma, and Cortez that evaluated a bypass water gas shift configuration for petroleum coke gasification units with co-production of 99% purity H<sub>2</sub>, employing an E-Gas gasifier<sup>1</sup>.

Previous studies<sup>2</sup> have shown that a conventional two-stage sour gas shift is capable of converting approximately 96% of CO initially in the syngas. A dual-stage Selexol unit that separates incoming CO<sub>2</sub> satisfies the 90% carbon capture requirement for that particular study. For systems that require less than 90% carbon capture, a reduced amount of CO can be shifted, or the Selexol unit can be downsized to capture less CO<sub>2</sub>. The former can be done by bypassing a portion of the raw syngas around the WGS section or by using less shift steam, and the latter by reducing column size, circulating less solvent, or bypassing a portion of syngas around the Selexol unit. This analysis maintains the same high performance dual-stage Selexol unit from the reference study<sup>2</sup>, and focuses strictly on methods to achieve lower degrees of CO shift by a combination of steam reduction, and syngas bypass around the shift reactors.

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<sup>i</sup> For this study, carbon capture is defined as carbon in the coal minus carbon leaving the stack. Any carbon that exits with the gasifier slag is not considered.

### 3 Conclusions and Recommendations

#### 3.1 Conclusions

The performance results for all cases considered are summarized in Table 1. The significant differences between cases are the number of shift stages used (one and two reactor configurations were considered) and the steam-to-dry-gas (S:DG) ratio assumed, which determines how much shift steam is required (both 0.3 and 0.25 S:DG ratios were evaluated). If shift steam levels are too low, the required reactor volume becomes prohibitively large, therefore negating the benefit of the steam savings.

**Table 1 - Water Gas Shift Case Results**

	<u>Case 1</u>	<u>Case 2</u>	<u>Case 3</u>	<u>Case 4</u>
<b><u>90% C Capture</u></b>				
• Number of stages	-	-	2	-
• S:DG <sup>ii</sup>	-	-	0.3	-
• LCOE, ¢/kWh	-	-	10.32	-
• System Efficiency, %	-	-	32.4	-
• Bypass, %	-	-	0	-
• Shift Steam, lb/hr	-	-	237,931	-
<b><u>85% C Capture</u></b>				
• Number of stages	-	-	2	2
• S:DG <sup>ii</sup>	-	-	0.3	0.25
• LCOE, ¢/kWh	-	-	10.17	10.10
• System Efficiency, %	-	-	32.9	33.2
• Bypass, %	-	-	8	7
• Shift Steam, lb/hr	-	-	216,575	163,952
<b><u>80% C Capture</u></b>				
• Number of stages	-	-	2	2
• S:DG <sup>ii</sup>	-	-	0.3	0.25
• LCOE, ¢/kWh	-	-	10.10	10.04
• System Efficiency, %	-	-	33.2	33.5
• Bypass, %	-	-	16	15
• Shift Steam, lb/hr	-	-	196,698	148,318
<b><u>75% C Capture</u></b>				
• Number of stages	1	1	2	2
• S:DG <sup>ii</sup>	0.3	0.25	0.3	0.25
• LCOE, ¢/kWh	10.05	9.97	10.01	9.97
• System Efficiency, %	33.3	33.6	33.5	33.7
• Bypass, %	6	2	24	23
• Shift Steam, lb/hr	145,751	90,382	175,981	132,782

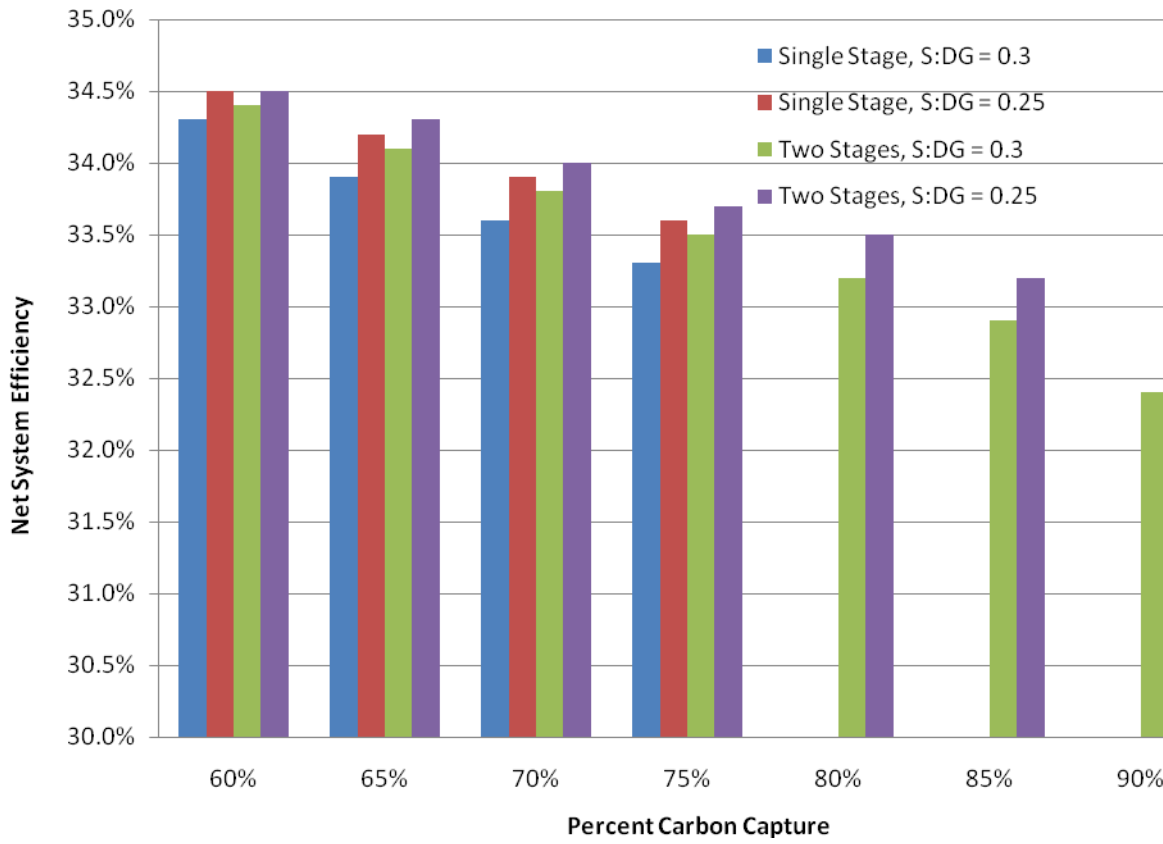
<sup>ii</sup> Steam to dry gas ratio is measured on a molar basis, at the outlet of the last shift reactor.



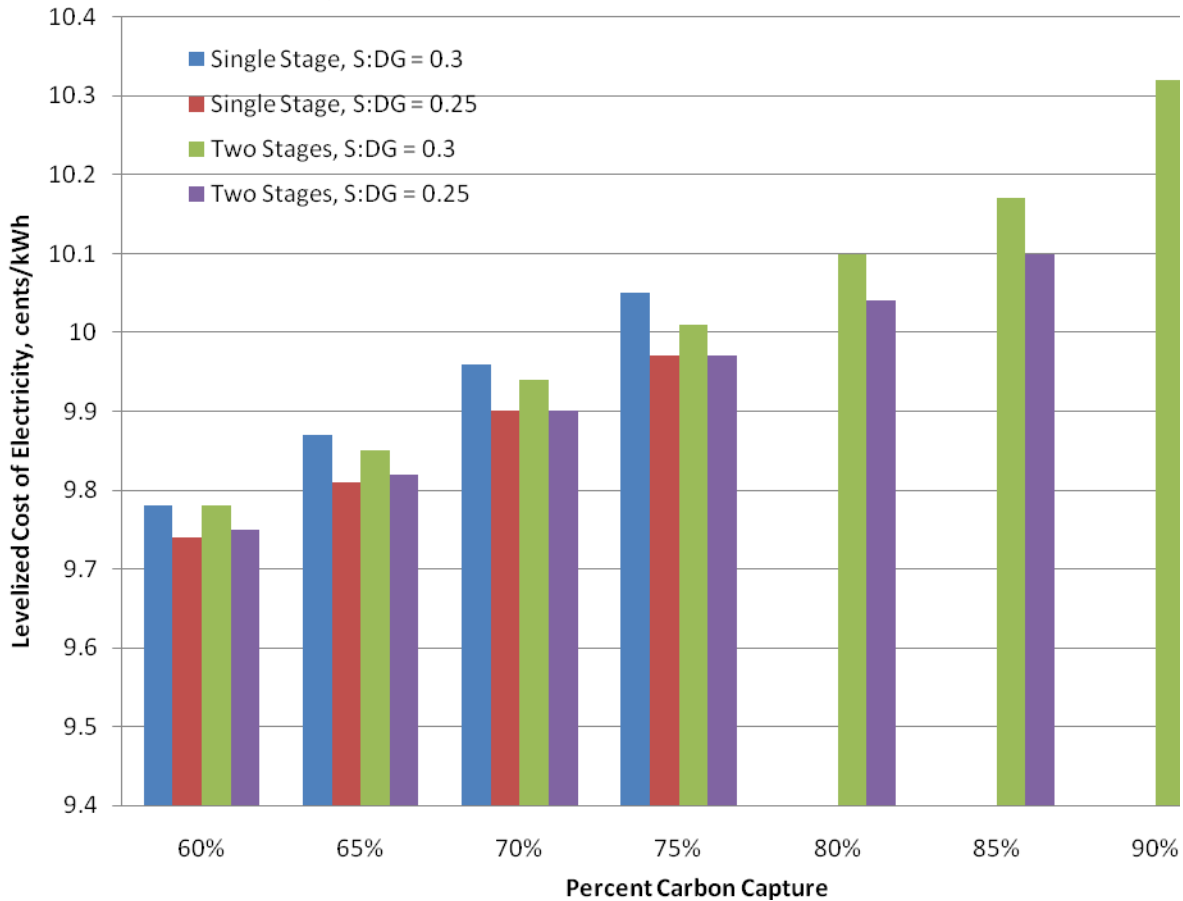
<b><u>70% C Capture</u></b>				
• Number of stages	1	1	2	2
• S:DG <sup>ii</sup>	0.3	0.25	0.3	0.25
• LCOE, ¢/kWh	9.96	9.90	9.94	9.90
• System Efficiency, %	33.6	33.9	33.8	34.0
• Bypass, %	16	13	33	32
• Shift Steam, lb/hr	129,672	80,138	155,834	117,009
<b><u>65% C Capture</u></b>				
• Number of stages	1	1	2	2
• S:DG <sup>ii</sup>	0.3	0.25	0.3	0.25
• LCOE, ¢/kWh	9.87	9.81	9.85	9.82
• System Efficiency, %	33.9	34.2	34.1	34.3
• Bypass, %	26	23	41	40
• Shift Steam, lb/hr	113,308	69,753	135,506	102,190
<b><u>60% C Capture</u></b>				
• Number of stages	1	1	2	2
• S:DG <sup>ii</sup>	0.3	0.25	0.3	0.25
• LCOE, ¢/kWh	9.78	9.74	9.78	9.75
• System Efficiency, %	34.3	34.5	34.4	34.5
• Bypass, %	37	34	49	48
• Shift Steam, lb/hr	96,341	60,007	116,089	88,067

Summaries of the efficiency and cost results for all cases are shown in Figure 1 and Figure 2, respectively. The results indicate that in general, there are efficiency and cost benefits when less shift steam is used (S:DG ratio of 0.25). For carbon capture below 75%, Figure 1 and Figure 2 indicate that the optimum configuration from an efficiency perspective uses two-stages and a steam-to-dry-gas ratio of 0.25. From a cost point of view, there is almost no difference if one or two shift stages are used for carbon capture below 75%, for the 0.25 S:DG cases. This result is counterintuitive, since there are two shift reactors (instead of one), but will be explained in more detail in later sections. Also of importance in Figure 1 and Figure 2 is that the maximum carbon capture possible with one shift reactor is 75%. The only configuration capable of meeting 90% carbon capture is two shift stages and a S:DG ratio of 0.3.

**Figure 1 - Water Gas Shift Case Efficiency Results**



**Figure 2 - Water Gas Shift Case Economic Results**



The following conclusions can be drawn from the results shown in Table 1, Figure 1, and Figure 2:

- For carbon capture greater than 75%, two water gas shift reactors are required. There is inadequate conversion of CO to CO<sub>2</sub> to achieve greater than 75% carbon capture if only one shift reactor is used.
- The maximum CO conversion in a single shift stage is approximately 75%. Therefore, the maximum carbon capture possible with only one shift reactor is also roughly 75%, depending on the separation efficiency of the Selexol unit, and the initial CO<sub>2</sub> content of the syngas (which is a function of the gasifier design).
- The most economic carbon capture design choice is to feed less shift steam (designing for a S:DG ratio of 0.25, instead of 0.3). Operating with a lower S:DG ratio impedes the kinetics of CO to CO<sub>2</sub> conversion. Consequently, larger and more costly WGS reactors are required for a similar degree of conversion. Although a reduction in S:DG ratio requires a larger reactor volume (this analysis assumed a volume increase of 30%, and subsequently a 30% increase in reactor cost), the benefit of steam savings – which can then be expanded through the steam turbine to produce additional power – is more than adequate to offset this.

- The only configuration capable of achieving 90% carbon capture (for the arrangement used in this analysis) is two reactor stages, with a S:DG ratio of 0.3. The maximum amount of shift steam is required in order to achieve high conversion of CO to CO<sub>2</sub>, which will allow for adequate Selexol separation to reach 90% capture.
- Figure 2 indicates that the COE of the single-stage configuration is the same as the two-stage configuration, for a steam-to-dry gas ratio of 0.25. This result is counterintuitive since there are fewer shift reactors, and according to Table 1 the steam consumption is also lower. The single stage configuration is not able to meet the sulfur emission limit (0.0128 lb SO<sub>2</sub>/MMBtu), since the WGS catalyst also promotes hydrolysis of carbonyl sulfide, according to the following reaction:

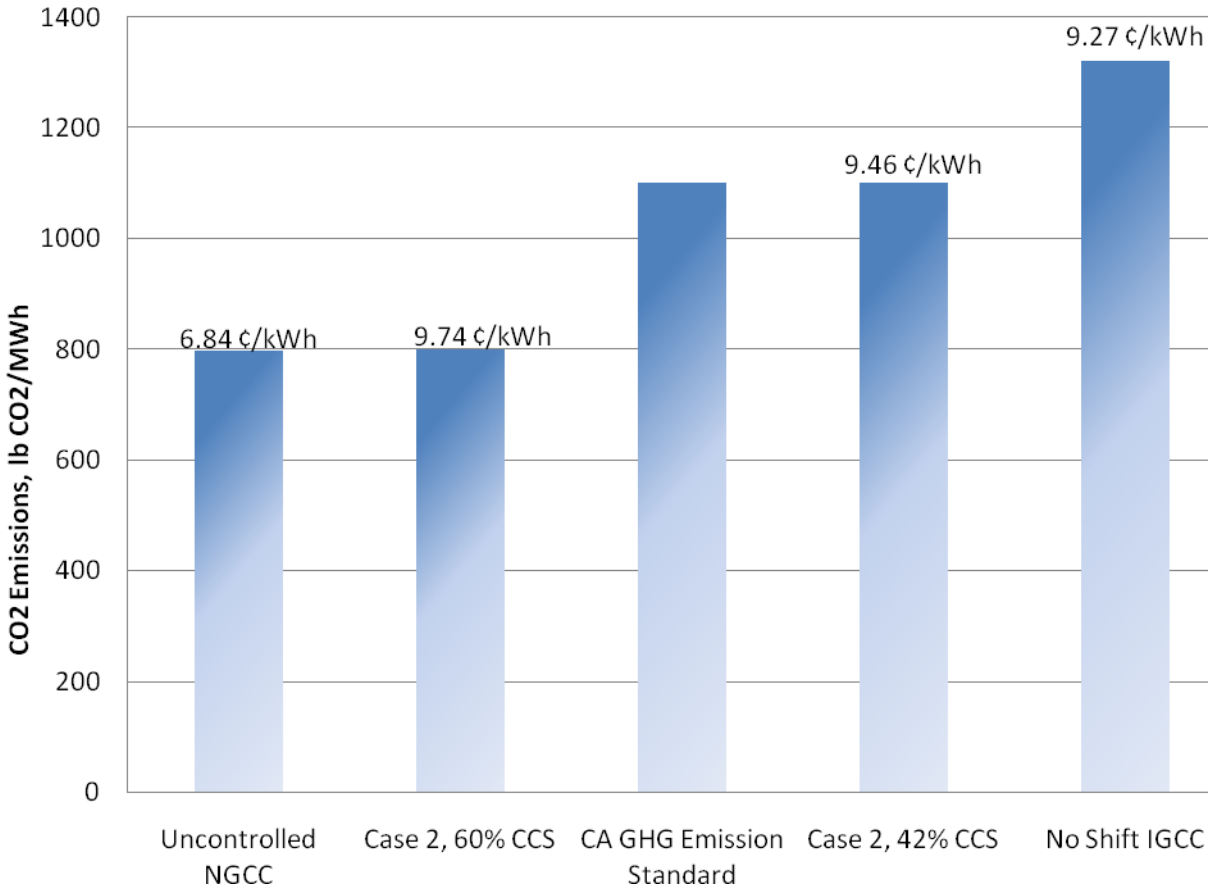


Therefore, although only one shift reactor is used, an additional carbonyl sulfide hydrolysis reactor is also required, which adds additional capital cost.

Figure 3 compares CO<sub>2</sub> emissions of an IGCC plant to an uncontrolled, advanced natural gas combined cycle (NGCC), and also to the emission limits of California's Senate Bill 1368, which requires the California Public Utility Commission to "establish a greenhouse gases emission performance standard for all baseload generation of local publicly owned electric utilities at a rate of emissions of greenhouse gases that is no higher than the rate of emissions of greenhouse gases for combined-cycle natural gas baseload generation<sup>3</sup>." This rate of emissions for a state-of-the-art NGCC has been established at 1,100 lb CO<sub>2</sub>/MWh.

An uncontrolled, advanced NGCC has a CO<sub>2</sub> emission rate of 800 lb CO<sub>2</sub>/MWh<sup>2</sup>, which is approximately equal to an IGCC plant capturing 60% of carbon emissions. On a cost basis, the IGCC plant at this emission rate is approximately 42% higher than the NGCC. To meet the California emission standard of 1,100 lb CO<sub>2</sub>/MWh, an IGCC plant would use a single shift stage, with 72% bypass around that reactor and a S:DG ratio of 0.25 to achieve 42% carbon capture, resulting in a cost of electricity of 9.46 ¢/kWh. The CO<sub>2</sub> emissions for an IGCC plant that did not shift CO, but captured carbon using a Selexol unit, are 1,322 lb CO<sub>2</sub>/MWh (29% carbon capture, 9.27 ¢/kWh).

**Figure 3 - CO<sub>2</sub> Emission Comparison**



### 3.2 Recommendations

For future IGCC designs, it is recommended that the water gas shift step be configured with larger reactors that are capable of operating with less shift steam. A typical commercial offering from a catalyst vendor recommends a S:DG ratio of at least 0.3 at the outlet of the last shift stage. However, discussions with vendors indicated that it may be possible to purchase reactors designed for a S:DG ratio of 0.25, although this would increase reactor volume by approximately 30%. It was assumed in this study that capital cost of the larger shift reactors would also increase by 30%. Therefore, this analysis explored the tradeoff between reduced shift steam consumption (reduced operating cost) and increased capital cost for the water gas shift step.

The results in Figure 2 show that for all levels of carbon capture, the cost of electricity is lowest when less shift steam is used. This trend suggests that although capital cost is higher due to larger reactors, the savings in shift steam consumption more than offsets this. For carbon capture below 75%, where a configuration using either one or two shift stages would be possible, the cost is nearly the same for either option. As explained

above, even though the single stage configuration has one less shift reactor, an additional COS hydrolysis reactor is required.

The efficiency results in Figure 1 show that when less shift steam is used (S:DG = 0.25), efficiency is higher, as expected. This is a direct result of more steam being expanded through the turbine to produce power, instead of being extracted and used for the water gas shift step. Figure 1 also shows that the efficiency of the two stage, 0.25 S:DG cases are higher than the single stage, 0.25 S:DG cases, even though the shift steam consumption is higher. In general, lower shift steam consumption would result in higher efficiency. When two shift stages are used instead of one, more syngas is bypassed around the reactor vessels. This leaves more exothermic reaction heat available for recovery and integration, since there is less mass present (shifted syngas) to absorb it. Therefore, when possible, it is recommended that two shift stages operating at a steam-to-dry-gas-ratio of 0.25 (at the reactor outlet) be used for future designs.

## **4 Base IGCC Case**

### **4.1 Plant Description**

The base IGCC plant for this analysis is Case 2 from the reference study<sup>2</sup>. This case is based on a 556 MWe (net power output) IGCC plant, using GE Energy gasification technology, located at a greenfield site in the Midwestern United States. The plant captures 90% of the carbon in the coal (minus carbon in the slag), and assumes geologic sequestration. Two pressurized, slurry-fed, entrained-flow gasification trains utilizing WGS reactors feed two advanced F-Class combustion turbines (rated at 232 MW each). Two heat recovery steam generators (HRSG's) and one steam turbine provide additional power. Carbon dioxide is removed with the two-stage Selexol physical solvent process. A block flow diagram of the process is shown in Figure 4.

Two gasification trains process a total of 6,005 tons of coal per day. Coal slurry is transferred from the slurry storage tank to the gasifier with a high-pressure pump. Ninety five percent purity oxygen is produced in a cryogenic air separation unit for use as the gasifier oxidant. The coal slurry and O<sub>2</sub> react in the gasifier at 815 psia and high temperature (in excess of 2,400°F) to produce syngas. Hot syngas and molten solids from the reactor flow downward into a radiant heat exchanger, where the syngas is cooled to 1,100°F and the ash solidifies. Raw syngas continues downward into a quench system, where most of the particulate matter is removed, and then into the syngas scrubber where the remaining entrained solids are separated along with halogens and ammonia. Slag captured by the quench system is recovered in a slag recovery unit. The gas is further cooled to accommodate cold cleanup processes, including a carbon bed for mercury removal.

To achieve the 90% carbon capture goal, a WGS process containing two intercooled sour shift stages operating at an inlet temperature of 450 °F converts CO to CO<sub>2</sub>. Carbon dioxide is removed from the cool, particulate-free gas stream by the Selexol solvent. The

dual-stage Selexol acid gas removal process preferentially removes hydrogen sulfide and carbon dioxide as purified product streams, which are sent for further processing. The H<sub>2</sub>S is converted to elemental sulfur in the Claus plant, and the CO<sub>2</sub> is dried and compressed to 2,215 psia for subsequent pipeline transport. The compressed CO<sub>2</sub> is transported via pipeline to a geologic sequestration field for injection into a saline aquifer, which is located within 50 miles of the plant.

A Brayton cycle, fueled by the sulfur- and relatively carbon-free syngas, is used in conjunction with a conventional subcritical steam-based Rankine cycle for combined-cycle power generation. The two cycles are integrated by generation of steam in the HRSG, and heat recovery from the IGCC process (radiant syngas cooler). A summary of plant electrical generation performance is presented in Table 2.

**Table 2 - GE IGCC Performance Summary**

Gas Turbine Power	464 MW
Steam Turbine Power	275 MW
Sweet Expander Power	6 MW
Auxiliary Power Requirement	(189 MW)
Net Power Output	556 MW
Net System Efficiency (HHV)	32.5%
Net Plant Heat Rate (HHV)	10,505 Btu/kWh

## 4.2 Plant Financial Description

Plant size, fuel type, design and construction time, total plant cost (TPC) basis year, plant capacity factor, heat rate, fuel cost, book life, and in-service date were used as inputs to develop capital cost, production cost, and LCOE estimates. Costs for the plant were based on adjusted vendor-furnished and actual cost data from recent design/build projects. Values for financial assumptions and a cost summary are shown in Table 3.

Project contingencies were added to each case to cover project uncertainty and the cost of any additional equipment that could result from detailed design. Process contingency is intended to compensate for uncertainties arising as a result of the state of technology development, and also was added to each plant section as appropriate. For more details on specific process and project contingencies as they were applied to each unit operation, the report containing the reference case should be consulted<sup>2</sup>.

The calculated cost of transport, storage, and monitoring for CO<sub>2</sub> is \$4.20/short ton, which adds 0.39 ¢/kWh to the LCOE.

**Table 3 - Base Case Financial Assumptions**

Capacity Factor	80%
Fuel Cost	\$1.80/MMBtu
Plant Life	30 years
Construction Duration	3 years

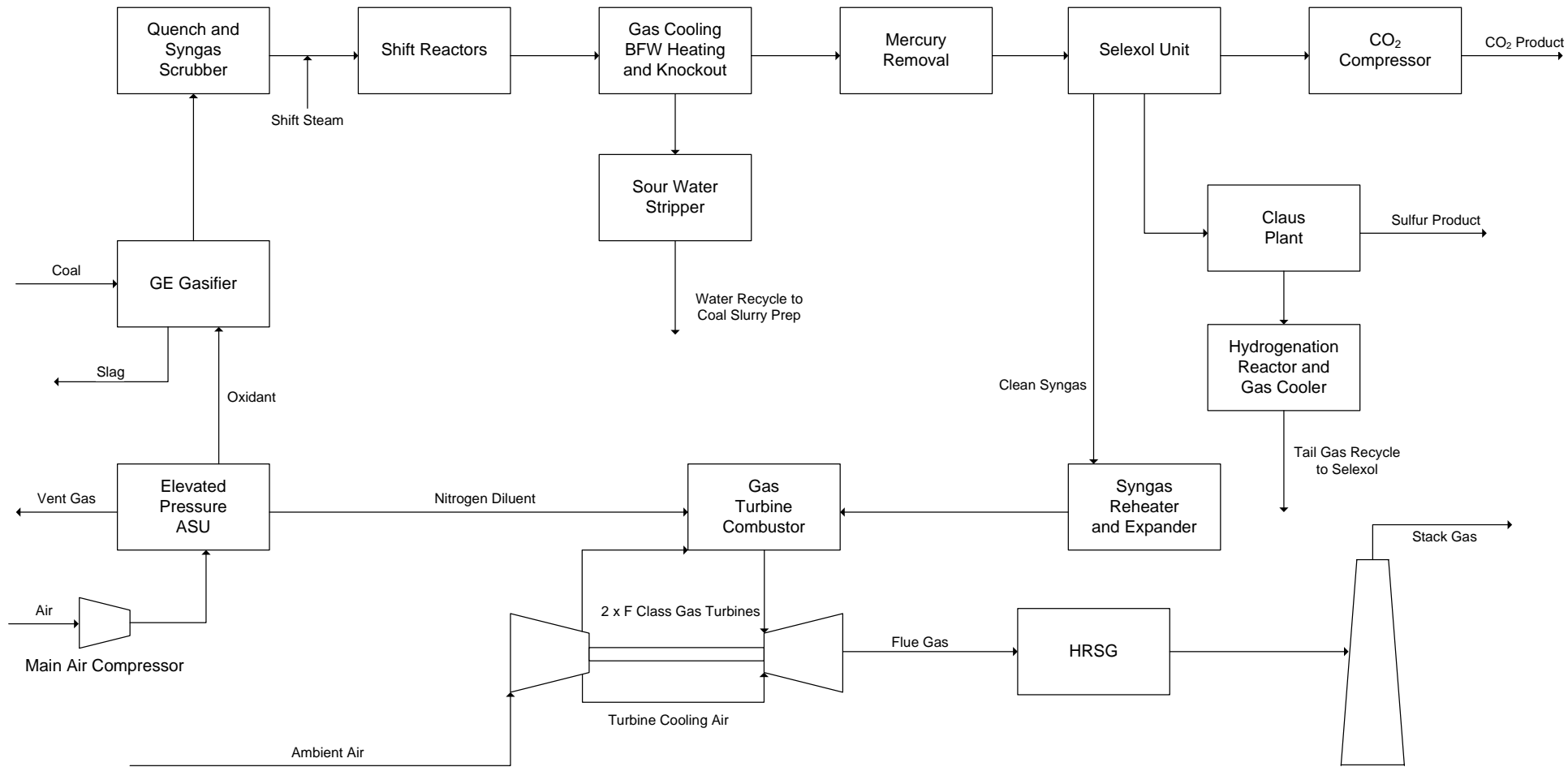
Plant in Service	January 2010
Capital Charge Factor	17.5%
Total Plant Cost <sup>iii</sup>	\$2,390/kWe
Levelized Cost of Electricity	10.29 ¢/kWh

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<sup>iii</sup>Total plant cost includes all equipment (complete with initial chemical and catalyst loadings), materials, labor (direct and indirect), engineering and construction management, and contingencies (process and project). Owner's costs are not included.



**Figure 4 - GE IGCC with Carbon Capture**



### 4.3 Base Case WGS Configuration

The water gas shift reaction produces CO<sub>2</sub> from CO, so that carbon is converted to a form that is more readily separated in an acid gas removal process such as a Selexol unit. The reaction consumes one mol of water per mol of CO converted, and releases heat in the process:



The sour water gas shift configuration for the base IGCC case is presented in more detail in Figure 5, and the corresponding stream data is in Table 4. It should be noted that this case is from the reference study<sup>2</sup>, and was specifically developed to capture 90% of carbon emissions.

The stream data in Table 4 show that the S:DG ratio at the outlet of the final shift reactor (stream 6) is 0.3. This represents a typical offering from a commercial catalyst vendor. The function of this excess steam is to drive the shift equilibrium toward the products.

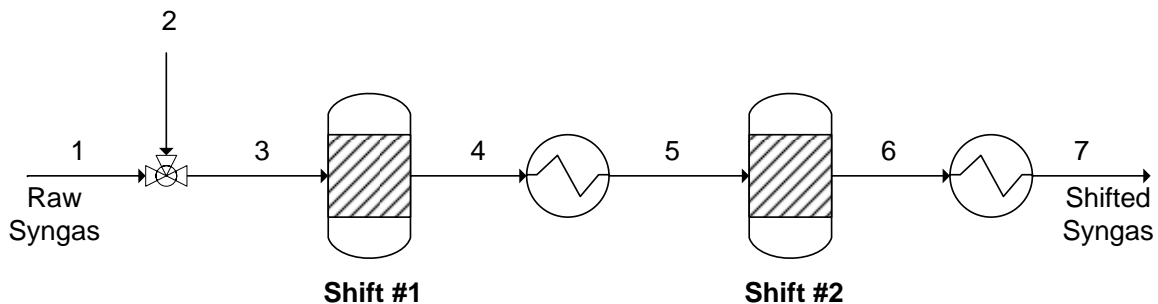
A secondary reaction that occurs on the WGS catalyst is hydrolysis of carbonyl sulfide:



This reaction converts sulfur to a form (H<sub>2</sub>S) that is removed more readily than COS in an acid gas removal system, helping to meet emission specifications. The Selexol solvent's affinity for H<sub>2</sub>S is nearly 4 times greater than it is for COS<sup>4</sup>. Since this physical solvent's driving force is partial pressure, and sulfur concentrations are relatively low to begin with, conversion to H<sub>2</sub>S (which the Selexol solvent can separate more easily) is effective in reducing the size of the Selexol process, while achieving the low sulfur levels required by local permitting agencies (this analysis assumes 0.0128 lb SO<sub>2</sub>/MMBtu).

The S:DG ratio used in this base case (0.3) represents a typical offering by a commercial catalyst vendor. The water gas shift and carbonyl sulfide hydrolysis reactions occur at locations within the catalyst matrix where water molecules have formed weak chemical bonds (chemisorption). These locations where the reactions occur are known as active sites. In order for chemisorption of water molecules to occur on the catalyst surface, diffusion of H<sub>2</sub>O through the bulk syngas must first occur. At the base case S:DG ratio, diffusion rates are fast enough such that there are adequate active catalyst sites on which the reactions can occur. This helps to maintain reasonable reactor sizes and costs.

**Figure 5 - Base Case Water Gas Shift Configuration**



**Table 4 - Base Case Water Gas Shift Stream Table**

Stream	1	2	3	4	5	6	7
Flow (lb/hr)	1,343,902	239,846	1,583,749	1,583,749	1,583,749	1,583,749	1,583,749
Temperature (°F)	410	615	446	801	450	519	450
Pressure (psia)	797.7	875.0	797.7	787.7	787.2	777.2	776.7
Enthalpy (MMBtu/hr)	-4393.6	-1324.6	-5718.2	-5717.9	-5963.6	-5963.6	-6011.3
H <sub>2</sub> mol %	0.26	0.	0.22	0.4	0.4	0.43	0.43
H <sub>2</sub> O mol %	0.34	1.	0.45	0.27	0.27	0.23	0.23
CO mol %	0.27	0.	0.22	0.04	0.04	0.01	0.01
CO <sub>2</sub> mol %	0.12	0.	0.1	0.28	0.28	0.31	0.31
H <sub>2</sub> S mol %	0.01	0.	0.	0.	0.	0.	0.
CH <sub>4</sub> mol %	0.	0.	0.	0.	0.	0.	0.
N <sub>2</sub> mol %	0.01	0.	0.01	0.01	0.01	0.01	0.01
Ar mol %	0.01	0.	0.01	0.01	0.01	0.01	0.01
Vapor Fraction	1.	1.	1.	1.	1.	1.	1.

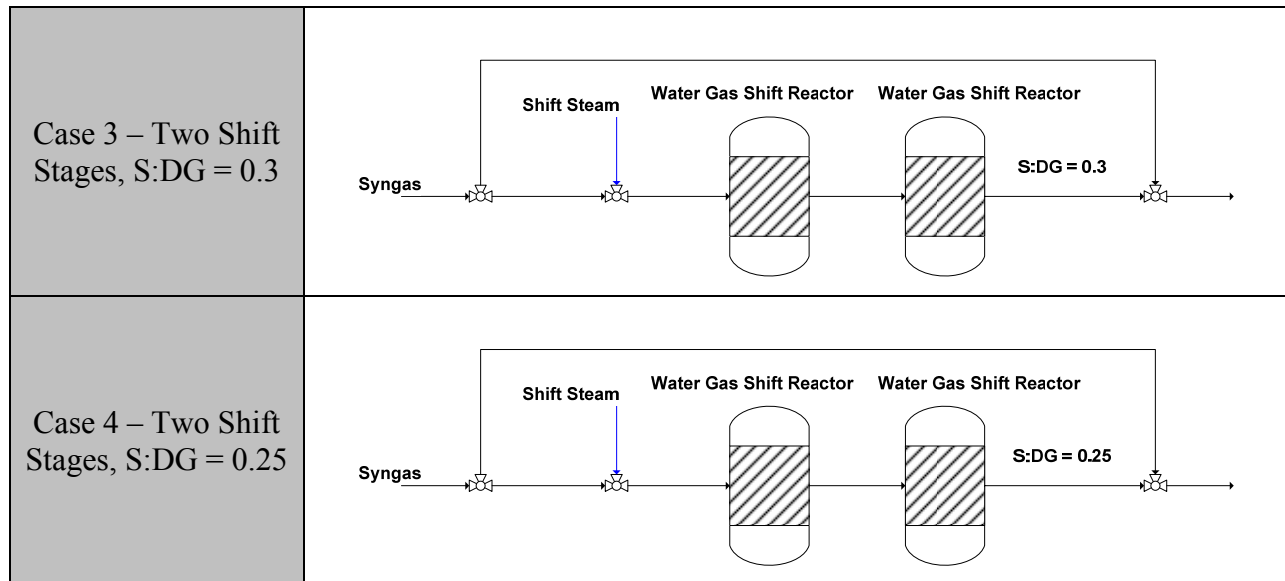
The purpose of this study is to optimize the water gas shift step for lower degrees of carbon capture (60-90%). The three methods that will be investigated are 1) to bypass a portion of syngas around the shift reactors, 2) to use less shift steam (a S:DG ratio of 0.25 will be used), and 3) to use one shift reactor instead of two. These will be used in combination with one another in order to arrive at the optimum configuration for each level of carbon capture.

## 5 Alternate Sour WGS Configurations

A simplified process flow diagram of each alternate water gas shift configuration is shown in Table 5. The technical and economic results of each configuration are shown in the following sections. The performance of each case was modeled using an AspenPlus 2004.1 simulation of an IGCC plant.

**Table 5 - Water Gas Shift Configuration Summary**

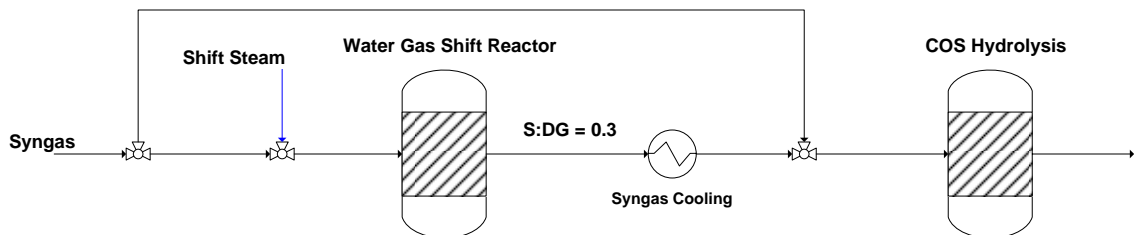
<p>Case 1 – Single Shift Stage, S:DG = 0.3</p>	
<p>Case 2 – Single Shift Stage, S:DG = 0.25</p>	



### 5.1 Case 1 - Single Shift Stage, S:DG = 0.3

Case 1 is characterized by a single shift stage, and fixed S:DG ratio of 0.3 at the reactor outlet. The bypass is set by the amount of CO conversion needed to meet the carbon capture goal. The maximum carbon capture possible with this configuration is approximately 75%. Since there is only one reactor used, the conversion of CO to CO<sub>2</sub> is limited to just over 70%. Given the relatively high CO<sub>2</sub> concentration of the syngas produced by a GE gasifier, 80% of the carbon present is in the form of carbon dioxide following a single stage of shift. Therefore, assuming a given Selexol performance, this configuration is capable of converting enough CO to CO<sub>2</sub> to achieve 75% capture of carbon dioxide for an IGCC plant that uses a GE gasifier<sup>iv</sup>. It is likely that this configuration will result in a different degree of capture when other gasifiers are used, since different gasifier models produce syngas streams with varying CO<sub>2</sub> levels. Performance of all other unit operations, including the Selexol process, was kept constant. Lower carbon capture targets (60-75%) were achieved by bypassing a portion of the syngas around a single shift reactor.

**Figure 6 - Case 1 Water Gas Shift Configuration**



This configuration requires an additional COS hydrolysis unit in order to achieve an emission rate of 0.0128 lb SO<sub>2</sub>/MMBtu. This is due to the syngas being bypassed around

<sup>iv</sup> Lower CO to CO<sub>2</sub> conversion will result in less overall carbon capture, since the Selexol solvent's affinity for CO<sub>2</sub> is approximately 19 times greater than it is for CO<sup>4</sup>.

the single shift reactor; the COS present is never hydrolyzed to H<sub>2</sub>S, and the Selexol solvent has less of an affinity for COS, resulting in higher total SO<sub>2</sub> emissions. This additional unit operation results in a capital cost increase.

The performance of the Case 1 WGS configuration over the range of carbon capture goals is shown in Table 6. The plant configuration and financial assumptions are the same as in the base case, with the exception of the water-gas shift section. The AspenPlus simulation results indicate that the upper carbon capture limit achievable with this configuration is 75%, with 6% bypass around the WGS reactor.

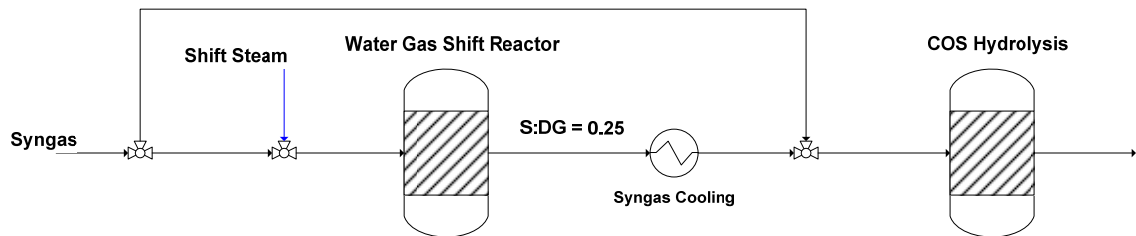
**Table 6 - Case 1 Performance Results**

Carbon Capture <sup>v</sup>	60%	65%	70%	75%
Syngas Shift Reactor Bypass	37%	26%	16%	6%
Gas Turbine Power (MW)	464	464	464	464
Steam Turbine Power	265	267	268	270
Sweet Gas Expander Power (MW)	6	6	6	6
Auxiliary Load (MW)	(177)	(179)	(181)	(183)
Net Power (MW)	558	558	557	556
Net System Efficiency (HHV)	34.3%	33.9%	33.6%	33.3%
Net Plant Heat Rate (Btu/kWh, HHV)	9,956	10,074	10,164	10,255
COE (¢/kWh)	9.78	9.87	9.96	10.05
Total Plant Cost (\$/kWe)	2,259	2,280	2,303	2,325

## 5.2 Case 2 - Single Shift Stage, S:DG = 0.25

The Case 2 configuration (shown in Figure 7) is identical to Case 1, except the shift steam is reduced such that the S:DG ratio is 0.25. The bypass around the shift reactor varies in order to achieve the specified degree of carbon capture. This alters the degree of CO to CO<sub>2</sub> conversion in order to achieve the specified carbon capture target. As in Case 1, an additional carbonyl sulfide hydrolysis reactor is required in order to meet the sulfur emission limit of 0.0128 lb SO<sub>2</sub>/MMBtu.

**Figure 7 - Case 2 Water Gas Shift Configuration**



As stated above, a typical commercial offering from a catalyst vendor requires a S:DG ratio of 0.3 in order to ensure an adequate number of active sites, keeping reactor size and cost low. While it may be theoretically possible to reduce this ratio, this will result in an increase in reactor size and cost. This cost increase represents a tradeoff with respect to

<sup>v</sup> All cases assume that the Selexol process removes 93% of the incoming CO<sub>2</sub>.

capital and operating costs: although capital cost increases due to a larger reactor, less shift steam will be consumed, lowering operating cost. This steam can then be expanded in the steam turbine to generate additional power. The Case 2 configuration is an examination of this tradeoff. The capital cost of the water gas shift island will be higher, but operating costs will be reduced.

The results for the Case 2 configuration are shown in Table 7. Similar to Case 1, this configuration is capable of no greater than 75% carbon capture due to the use of only one reactor. In addition, the low shift steam does not drive the reaction equilibrium toward the products (H<sub>2</sub> and CO<sub>2</sub>) as aggressively as in Case 1, which had higher steam consumption.

**Table 7 - Case 2 Performance Results**

Carbon Capture <sup>vi</sup>	60%	65%	70%	75%
Syngas Shift Reactor Bypass	34%	23%	13%	2%
Gas Turbine Power (MW)	464	464	464	464
Steam Turbine Power	270	271	272	275
Sweet Gas Expander Power (MW)	6	6	6	6
Auxiliary Load (MW)	177	179	181	183
Net Power (MW)	562	562	561	561
Net System Efficiency (HHV)	34.5%	34.2%	33.9%	33.6%
Net Plant Heat Rate (Btu/kWh, HHV)	9,899	9,985	10,074	10,164
COE (¢/kWh)	9.74	9.81	9.90	9.97
Total Plant Cost (\$/kWe)	2,248	2,269	2,290	2,310

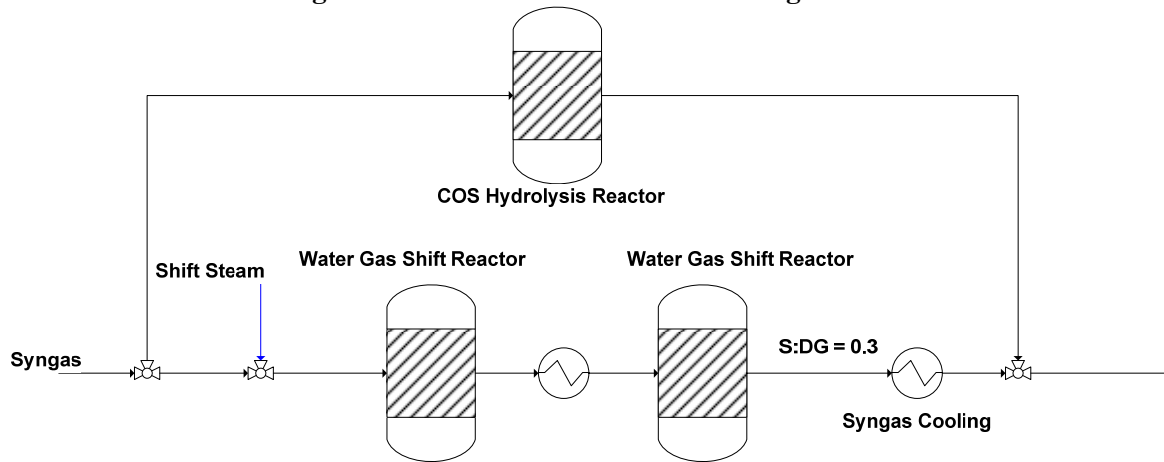
The results in Table 7 show a slight cost and performance advantage for Case 2. This suggests that although the larger shift reactors result in increased capital cost, this is more than offset by the savings in shift steam consumption.

### 5.3 Case 3 - Two Shift Stages, S:DG = 0.3

The Case 3 configuration, shown in Figure 8, is based on a two stage system, with a portion of the syngas bypassing both stages. It is the same as Case 1, except with a second stage added. The addition of the second stage will allow for greater CO conversion, given the same bypass rate and supplemental steam consumption. The process tradeoff with this configuration is the requirement of an external COS hydrolysis reactor; although carbon capture is achievable with greater bypass rates, the COS in the bypass stream is never hydrolyzed in the shift reactors, contributing to greater sulfur emissions. The supplemental steam flow is regulated such that the steam-to-dry gas ratio is 0.3 at the outlet of the second shift stage.

<sup>vi</sup> All cases assume that the Selexol process removes 93% of the incoming CO<sub>2</sub>.

**Figure 8 - Case 3 Water Gas Shift Configuration**



The Case 3 performance results are shown in Table 8. This configuration has the benefit of being able to accommodate the entire range of carbon capture targets considered in this study. With high syngas bypass rates, an external COS hydrolysis reactor is required to achieve the sulfur emission limit of 0.0128 lb SO<sub>2</sub>/MMBtu. However for the 85% and 90% capture cases, enough hydrolysis occurs directly on the shift catalyst such that the additional reactor is not required.

**Table 8 - Case 3 Performance Results**

Carbon Capture	60%	65%	70%	75%	80%	85%	90%
Syngas Bypass	49%	40%	32%	23%	15%	7%	0%
Gas Turbine Power (MW)	464	464	464	464	464	464	464
Steam Turbine Power	267	269	270	272	273	275	275
Sweet Gas Expander Power (MW)	6	6	6	6	6	6	6
Auxiliary Load (MW)	(177)	(179)	(181)	(183)	(186)	(188)	(189)
Net Power (MW)	560	560	559	559	558	557	556
Net System Efficiency (HHV)	34.4%	34.1%	33.8%	33.5%	33.2%	32.9%	32.4%
Net Plant Heat Rate (Btu/kWh, HHV)	9,927	10,015	10,104	10,194	10,286	10,380	10,540
COE (¢/kWh)	9.78	9.85	9.94	10.01	10.10	10.17	10.32
Total Plant Cost (\$/kWe)	2,259	2,279	2,300	2,320	2,341	2,356	2,390

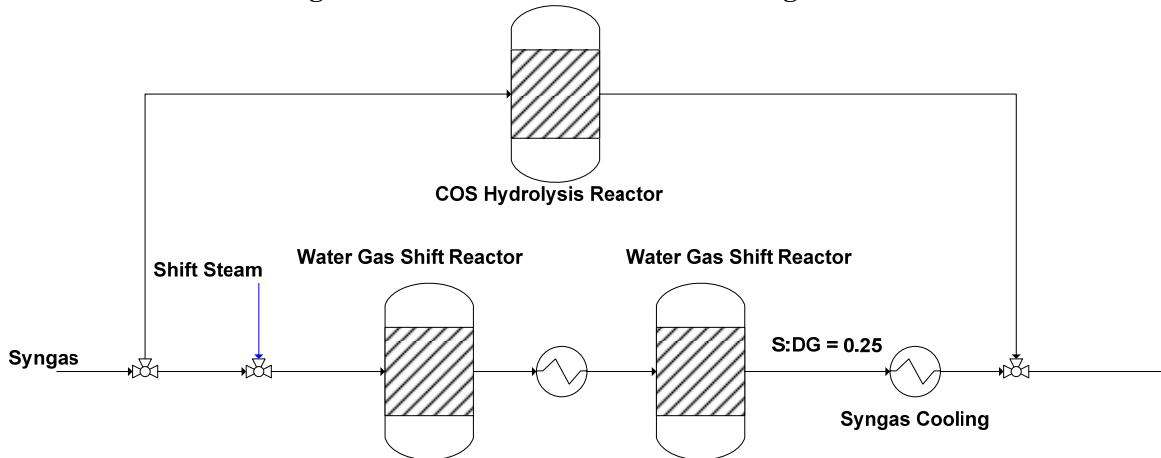
Comparing the Case 3 results with those from Case 1 shows the cost and performance differences associated with the addition of a second shift reactor, at an identical steam-to-dry gas ratio (in this instance, 0.3). Although there is more capital equipment for the two-stage arrangement, this configuration resulted in higher efficiency, and lower cost. The addition of the second shift reactor allowed for greater bypass rates to achieve the same level of capture. Therefore, since there is less syngas mass being shifted, greater reaction heat recovery is possible between stages (more mass being shifted would result in an increase in the temperature of the shifted syngas, and less heat available for recovery). This heat is integrated into the HRSG, allowing for greater steam turbine power output. A comparison of the Case 3 steam turbine power output to Case 1 (Table 9) shows greater steam cycle power output for all levels of carbon capture.

**Table 9 - Steam Cycle Power Comparison**

Carbon Capture	60%	65%	70%	75%
Case 1 Steam Cycle Power, MW	265	267	268	270
Case 3 Steam Cycle Power, MW	267	269	270	272

#### 5.4 Case 4 - Two Shift Stages, S:DG = 0.25

The Case 4 configuration, shown in Figure 9, is based on a two stage system, with a portion of the syngas bypassing both stages. The steam-to-dry gas ratio is reduced in this case, using the 0.25 S:DG metric. Although this results in larger shift reactors, and subsequently increased capital cost, a shift steam savings is realized. Similar to Case 3, this configuration requires an external COS hydrolysis reactor; although carbon capture is achievable with greater bypass rates, the COS in the bypass stream is never hydrolyzed in the shift reactors, contributing to greater sulfur emissions.

**Figure 9 - Case 4 Water Gas Shift Configuration**

The Case 4 performance results are shown in Table 10. This configuration is capable of meeting the entire range of carbon capture targets, with the exception of the 90% capture case. This suggests that to achieve 90% carbon capture, not only are two shift stages required, but high shift steam use is also needed to drive the reaction equilibrium toward the products ( $H_2$  and  $CO_2$ ). With high syngas bypass rates, an external COS hydrolysis reactor is required to achieve the sulfur emission limit of 0.0128 lb  $SO_2$ /MMBtu. However for the 85% capture case, adequate hydrolysis occurs directly on the shift catalyst such that the additional reactor is not required.

**Table 10 - Case 4 Performance Results**

Carbon Capture	60%	65%	70%	75%	80%	85%
Syngas Bypass	48%	40%	32%	23%	15%	7%
Gas Turbine Power (MW)	464	464	464	464	464	464
Steam Turbine Power	270	272	274	277	278	281
Sweet Gas Expander Power (MW)	6	6	6	6	6	6
Auxiliary Load (MW)	(177)	(179)	(181)	(183)	(185)	(188)
Net Power (MW)	563	563	563	563	563	563



Net System Efficiency (HHV)	34.5%	34.3%	34.0%	33.7%	33.5%	33.2%
Net Plant Heat Rate (Btu/kWh, HHV)	9,899	9,956	10,044	10,134	10,194	10,286
COE (¢/kWh)	9.75	9.82	9.90	9.97	10.04	10.10
Total Plant Cost (\$/kWe)	2,257	2,275	2,294	2,311	2,330	2,342

A comparison of the Case 3 and Case 4 results is presented in Table 11. This shows the performance changes associated with a reduction in shift steam consumption (from a steam-to-dry gas ratio of 0.3 in Case 3 to 0.25 in Case 4). Since less shift steam is consumed in Case 4, steam cycle power increases, and the system efficiency also increases. As explained earlier, a reduction in shift steam requires larger reactor sizes, which increases capital cost. Despite this capital cost increase, the savings in shift steam consumption was great enough to result in a lower levelized cost of electricity. However, the Case 4 configuration was not capable of achieving enough water gas shift to meet the 90% carbon capture target. This suggests that the incremental shift that allows for meeting elevated (90% or greater) carbon capture is due to high shift steam consumption (a steam-to-dry gas ratio of 0.3).

**Table 11 - Two Stage Shift Comparison**

Carbon Capture	Case 3 Steam Cycle Power, MW	Case 3 Efficiency	Case 3 LCOE, ¢/kWh	Case 4 Steam Cycle Power, MW	Case 4 Efficiency	Case 4 LCOE, ¢/kWh
60%	267	34.4%	9.78	270	34.5%	9.75
65%	269	34.1%	9.85	272	34.3%	9.82
70%	270	33.8%	9.94	274	34.0%	9.90
75%	272	33.5%	10.01	277	33.7%	9.97
80%	273	33.2%	10.10	278	33.5%	10.04
85%	275	32.9%	10.17	281	33.2%	10.10

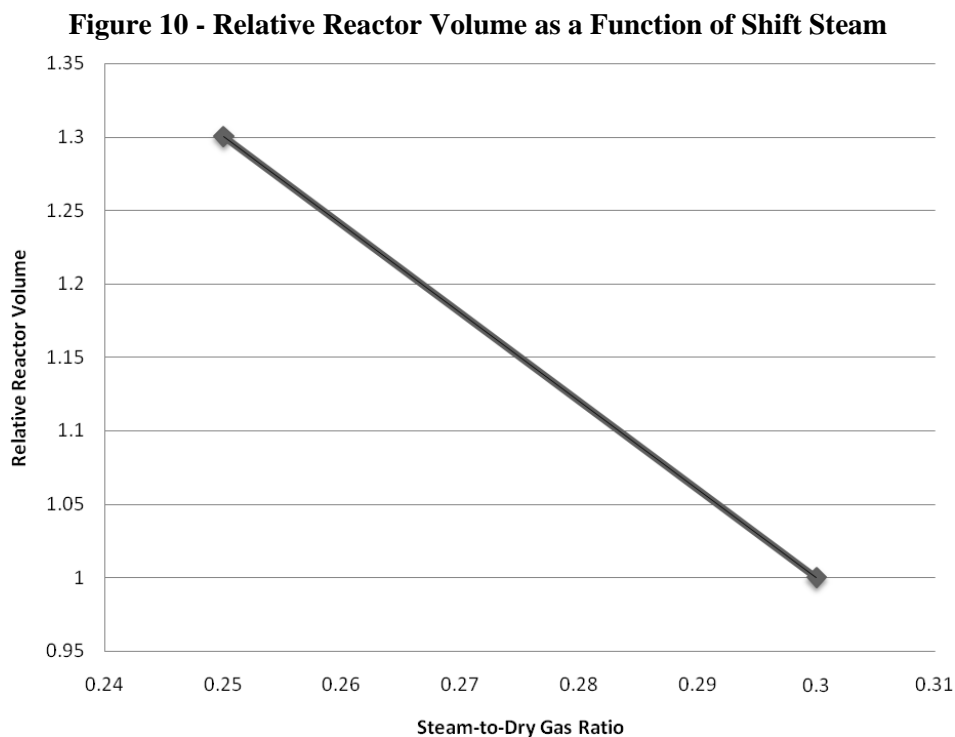
## 6 Shift Reactor Design Considerations

### 6.1 Steam-to-Dry Gas Ratio

The S:DG ratio used in the base case (0.3) represents a typical offering by a commercial catalyst vendor. The water gas shift and carbonyl sulfide hydrolysis reactions occur at locations within the catalyst matrix where water molecules have formed weak chemical bonds (chemisorption). These locations where the reactions occur are known as active sites. In order for chemisorption of water molecules to occur on the catalyst surface, diffusion of H<sub>2</sub>O through the bulk syngas must first occur. At the base case S:DG ratio, syngas water concentration is high enough to allow for relatively fast diffusion rates. This ease of diffusion of water through the bulk syngas and onto the catalyst surface results in an adequate number of active catalyst sites on which the reactions can occur. This helps to maintain reasonable reactor sizes and costs.

While it is technically possible to achieve comparable levels of CO conversion with less shift steam, this will require larger reactor sizes. Fewer water molecules in the syngas will result in slower diffusion of H<sub>2</sub>O through the bulk syngas, and onto the catalyst surface to

form active reaction sites. Therefore, more catalyst surface must be provided to maintain the same level of CO conversion. This analysis assumes that a reduction in S:DG from 0.3 to 0.25 requires 30% additional reactor volume<sup>5</sup>, and subsequently 30% cost increase. This trend is shown graphically in Figure 10.



## 6.2 Water Gas Shift Reactor Pressure Drop

Typical catalyst size for water gas shift service utilizes particles in the range of 3 to 10 mm in diameter. Since the WGS reactors are typically packed beds, the Ergun equation, shown below, can be employed to calculate the pressure drop<sup>6</sup>:

Equation 1 – Ergun Equation for Pressure Drop Through Packed Beds

$$\frac{\Delta P}{L} = \frac{\rho_f u^2}{g d_p \phi} \cdot \frac{(1 - \varepsilon)}{\varepsilon^3} \cdot \left[ 150 \frac{(1 - \varepsilon)}{\phi (\text{Re})_p} + 1.75 \right]$$

Where

$d_p$  = particle diameter

$g$  = gravitational acceleration

$L$  = bed length

$\Delta P$  = pressure drop

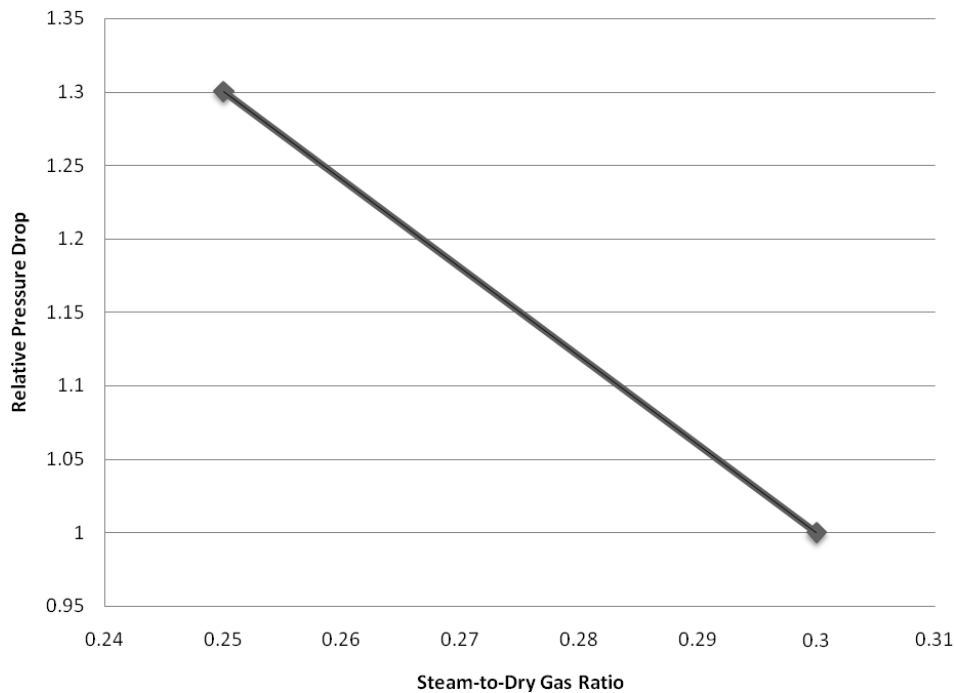
$(\text{Re})_p$  = particle Reynolds number =  $\frac{d_p u \rho_f}{\mu}$

$u$  = superficial fluid velocity

- $\phi$  = particle shape factor
- $\varepsilon$  = packed bed voidage
- $\rho_f$  = fluid density
- $\mu$  = fluid viscosity

Once all the parameters are known, the pressure drop can be calculated from Equation 1. Since some of the operating conditions of the current WGS reactors have not been selected, detailed calculations of reactor pressure drop can not be performed. However, relative pressure drop changes versus the operating S:DG molar ratios can be evaluated easily. Given the same operating pressure, velocity, and catalyst, the pressure drop is proportional to the length of the reactor. Given the increase in size (length) due to reduced shift steam consumption (established in the previous section), the relative pressure drop can also be calculated. This is shown graphically in Figure 11.

**Figure 11 - Relative Reactor Pressure Drop as a Function of Shift Steam**



## 7 Water Gas Shift Background

### 7.1 Steam Consumption

In order to drive the reaction equilibrium toward the products, an excess of steam is typically introduced at the shift stage inlet. Depending on the gasifier type (slurry versus dry feed, or firetube boiler versus syngas water quench) there can be insufficient water vapor initially present in the syngas, so steam is usually extracted from the steam bottoming cycle and introduced to the shift process. Therefore, the WGS reaction is usually viewed as a burden on the net system efficiency, due to steam withdrawal.

## 7.2 Sweet Versus Sour Shift

There are two concepts for shifting coal-derived syngas, a sweet shift and a sour shift, the difference being the sulfur level in the syngas. The feed to a sweet shift unit must be sulfur free, due to the poisonous effects of sulfur on the catalyst used for this application. For coal-derived syngas, sulfur is typically removed by a cold-gas cleaning system such as a single-stage Selexol unit. The catalyst used for a sour shift is sulfur tolerant, so no scrubbing is required upstream of the reactor.

Since the WGS reaction is exothermic, a low temperature regime is thermodynamically favored for driving the reaction toward the products; however, the reaction kinetics favor high temperature. This competition between thermodynamics and kinetics results in the reaction being executed in a series of steps, with intercooling between each reactor, to achieve high CO conversion. The exact number of steps will depend on the degree of conversion required to achieve the CO<sub>2</sub> capture target, as well as the specific catalyst being used. For IGCC applications where 90% CO<sub>2</sub> capture with a cold process (such as Selexol) is required, typically two (and sometimes three) reactors are used. Table 12 compares operating temperatures and CO slip for three-stage sweet and sour shifts.

The values in Table 12 show an operating tradeoff between the two shift options: although a sour shift catalyst is sulfur tolerant, eliminating the capital expenditure associated with syngas precleaning, it does require lower operating temperatures, which increases irreversible heat loss in the system. Therefore, the decision that chooses a shift scenario (sweet versus sour) will balance capital with operating costs.

**Table 12 - Sweet and Sour Shift Comparison<sup>7</sup>**

	Reactor Temperature, °F		CO Slip, mol % (dry)	
	Sweet Shift	Sour Shift	Sweet Shift	Sour Shift
<b>1<sup>st</sup> Reactor</b>	662	554	6.41	4.43
<b>2<sup>nd</sup> Reactor</b>	662	608	2.12	1.77
<b>3<sup>rd</sup> Reactor</b>	464	608	0.48	0.88

### 7.2.1 Sweet Shift

The syngas feed to the WGS reactor must be nearly sulfur-free (0.1 ppmv<sup>1</sup>) for a sweet shift configuration, requiring an acid gas removal (AGR) system. If a conventional cold gas cleanup process is used for sulfur removal, the water vapor present in the syngas will condense during cooling prior to the AGR. Therefore, if a sweet shift is paired with a cold gas cleanup process (such as Selexol), the syngas feed to the shift reactor will be nearly moisture-free.

Any water initially present in the syngas that is condensed out due to cooling will have to be supplemented by steam extracted from the bottoming cycle (to drive the shift equilibrium), resulting in greater efficiency losses. Therefore, a sweet gas shift may not be the optimum choice for a syngas stream rich in water vapor, such as that produced from a slurry-fed gasifier or direct water quench.

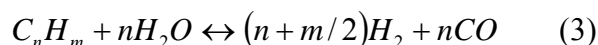
A sweet shift may be better paired with a dry fed gasifier, which produces syngas with lower moisture levels than slurry fed gasifiers. Since there is less moisture present to begin with, the efficiency loss associated with condensation and subsequent steam addition would be minimized. Another sweet shift application may be for cogeneration systems, which produces syngas for power, as well as hydrogen. Since the hydrogen requires low moisture levels, cold gas cleaning prior to a sweet shift may be an option for water removal.

### 7.2.2 Sour Shift

For IGCC applications with carbon capture, a sour shift may be a better fit due to the sulfur tolerance of the catalyst. An IGCC system that uses a slurry-fed gasifier will produce syngas with high moisture content. The high water vapor concentration of the syngas provides a strong partial pressure driving force for the shift equilibrium, with lesser amounts of supplemental steam required from the bottoming cycle. A sour shift will promote moisture retention in the vapor phase because there is no upstream cold sulfur removal required. This would eliminate the need for upstream cold gas cleaning, and the subsequent water vapor condensation associated with a cold process.

## 7.3 WGS Reaction Equilibrium and Stage Operation

Water gas shift reactors are generally used in the industrial production of hydrogen, ammonia, and other bulk chemicals employing synthesis gases. In the catalytic steam reforming of hydrocarbons, the following general chemical equation applies<sup>8</sup>:



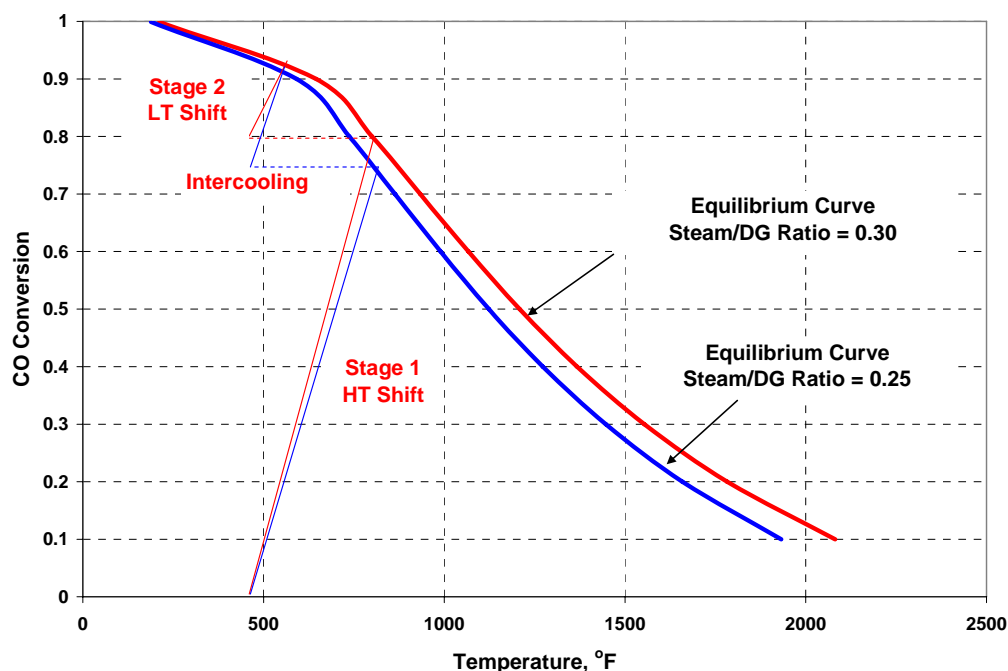
The water-gas shift reaction also occurs in the reformer. In industrial applications the reforming and shift reactions result in a product with compositions closely approaching equilibrium. The reformers and the shift converters are fixed bed catalytic reactors. In order to drive the reaction equilibrium toward the products, excess steam is used. The reactions do not approach completion in the reformers, usually with 10-15 volume percent CO in the reformer effluent (dry basis). Further conversion of CO is carried out using water gas shift reactors to reduce the concentration of CO to about 0.5-1% (5,000-10,000 ppmv). Depending on the synthesis requirements of the purified syngas, the ratio of CO and H<sub>2</sub> is adjusted via the water gas shift reaction. For example, hydrogen production or ammonia synthesis typically requires maximum H<sub>2</sub> yield. For methanol synthesis, a H<sub>2</sub> to CO ratio of 2:1 is required. The water gas shift reaction can achieve nearly any desired stoichiometry by bypassing part of the total gas stream and shifting only a portion of it. For IGCC application, the primary objective of the water gas shift step is to convert CO to CO<sub>2</sub> for subsequent removal and sequestration.

The water-gas shift reaction is equilibrium limited and moderately exothermic (-17,697 Btu/lb-mol). Its equilibrium constant decreases with increases in temperature, therefore high conversion is favored at low temperature. Low CO levels can only be achieved at low temperatures or driven thermodynamically by excess steam, even though the kinetics are more favorable at higher temperatures. Thus, in order to achieve lower equilibrium CO levels, two or three WGS reactors are typically employed in industry: a high-temperature shift (HTS)

reactor, operating between 644°F (340°C) and 986°F (530°C), for rapid CO conversion, and one or two low-temperature shift (LTS) reactors, operating between 356°F (180°C) to 446°F (230°C). In commercial applications, adiabatic fixed bed reactors with inter-reactor quenching are usually used<sup>9</sup>. The inter-reactor quenching can be accomplished by two ways, direct and indirect quenching. The indirect cooling makes use of cooling tubes while the direct cooling employs direct water quench. The direct water quench requires less capital investment but is less efficient in the recovery of reaction heat.

With a given feed composition, the equilibrium conversion of the WGS reaction can be determined. It can be verified that for very low exiting CO concentration, either low temperature, high water content, or some combination of both are required. Under adiabatic conditions, the conversion in a single bed is thermodynamically limited because the reactor operating temperature increases as the reaction proceeds. Therefore, to increase conversion, more than one reactor with intercooling between stages is usually employed. Figure 12 shows graphically the two-stage WGS adiabatic reactor system with intercooling for syngas compositions with S:DG molar ratios of 0.3 and 0.25. The figure also shows that the equilibrium compositions are calculated at the adiabatic exit temperature of the reactors, consistent with the current AspenPlus simulation program.

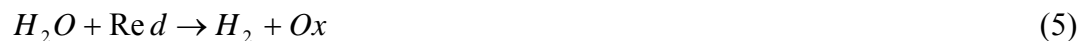
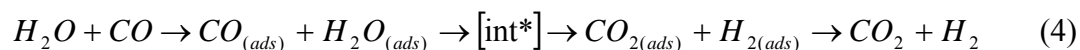
**Figure 12 - Two Stage WGS Reactor Operation with Intercooling**



## 7.4 WGS Reaction Kinetics

Although numerous studies of reaction kinetics and mechanisms for the water gas shift reaction have been reported in the literature, there is still controversy over the reaction mechanism, the active reaction site, and the effect of pressure<sup>10</sup>. This disagreement was attributed to the presence of impurities, the varying degrees of mass transfer limitations, the different types of catalysts employed, and the fact that most of the experimental reactors operate at or close to atmospheric pressure.

For the HTS catalyst such as iron oxide/chromia, there are two distinctly different kinetic mechanisms which were proposed: the “adsorptive mechanism” (4) and the “regenerative mechanism” (5 and 6).



Red represents a reduced site and Ox, an oxidized site. In the adsorptive mechanism (4), CO and H<sub>2</sub>O first adsorb onto the catalyst surface and form an intermediate. Subsequent desorption results in desorbed hydrogen and CO<sub>2</sub>. In the regenerative mechanism (5), water first adsorbs and dissociates on a reduced site of catalyst surface to produce hydrogen and at the same time, it oxidizes the site. In the following step (6) CO is oxidized to CO<sub>2</sub> at this site.

In contrast to rate expressions from detailed reaction mechanisms and rate determining steps, there are also simple empirical rate expressions proposed which do not consider any mechanism. Other research groups recognize that the water-gas shift reaction is not a simple order reaction, especially at higher steam:CO ratios, and have suggested a power-law type of kinetic equation.

For adiabatic reactors, the rate equation needs to be integrated from the reactor inlet to the outlet, a very tedious effort only justified for detailed WGS reactor design. For routine design, it is recommended to evaluate the equilibrium constant,  $K_{eq}$ , at the outlet temperature of the reactor and calculate the rate constant,  $k$ , as an arithmetic average of rates at the inlet and outlet temperatures<sup>11</sup>.

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