A Technical and Economic Assessment of Selexol-based CO_2 Capture Technology for IGCC Power Plants

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Chao Chen
Advisor: Edward S. Rubin

Abstract

Increasing CO_2 emissions and concerns about potential climate change are arousing great interest in the technical and economic feasibility of capturing CO_2 from large energy system, such as coal-based power plants. Performance and cost models of a Selexol-based CO_2 absorption system for capturing CO_2 from an advanced power system (Integrated Gasification Combined Cycle, IGCC) have been developed and integrated with an existing IGCC modeling framework without CO_2 capture. The integrated model has been applied to study the feasibility, cost and uncertainties of carbon capture and sequestration at both greenfield and repowered IGCC plants. The analysis shows that based on commercially available technology, the cost of CO_2 avoided for an IGCC power plant is half that for a conventional combustion plant with a chemical absorption process. For IGCC systems, the uncertainty associated with CO_2 transport and storage has the largest impact on the cost of CO_2 avoided. Under suitable conditions, IGCC repowering was shown to be an attractive option for reducing CO_2 emissions from existing coal-fired plants. Compared to building greenfield IGCC plants, IGCC repowering also provides an option for introducing new power generation technology with lower risk to utilities.

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Introduction

The possibility of global climate change resulting from increasing levels of greenhouse gases, including carbon dioxide (CO_2), is the subject of considerable debate and uncertainty [1-2], but the increasing atmospheric concentration of CO_2 could have significant impacts that may not be easily reversed [3]. The combustion of fossil fuel to produce power is a major source of industrial CO_2 emissions [4]. Hence, limiting CO_2 emission from large-scale fossil fuel-based power plants might be a key element of a strategy for sustainable development. The primary strategies under consideration include the increasing use of non-fossil energy sources and, more recently, capturing and sequestering of CO_2 from fossil fuels [5-7], especially from coal for the reasons explained below. Regardless of the future of non-fossil energy sources, such as nuclear energy and renewable energy, coal will certainly be one of the major fuels for power generation because in comparison to other fossil fuels, coal is characterized by rich reserves and low prices. On the other hand, coal is also known as a dirty and high-carbon intensive energy source. This scenario has generated substantial interest in developing a coal utilization technology that minimizes the production of greenhouse gases as well as conventional pollutants SO_2, NO_x, and particulates.

An emerging coal-based technology, Integration Gasification Combined Cycle (IGCC) system is becoming an increasingly attractive option to limit CO_2 emission and other pollutants relative to conventional coal power plants because of its several desired attributes. First, IGCC systems provide relatively high energy conversion efficiency, with the prospect of even higher efficiencies if higher temperature gas turbines and hot gas cleanup systems are employed. Second, IGCC has a technology cleanup advantage compared to conventional combustion-based coal plants. The reducing atmosphere of a gasifier alters the chemical form of pollutants, and it is inherently easier to remove hydrogen sulfide (H_2S) and ammonia (NH_3) from a pressurized fuel gas stream produced by a gasifier than to remove sulfur oxides (SO_x) and nitrogen oxides (NOx) from an atmospheric exhaust stream from a boiler. In fact, very low emission levels for sulfur and nitrogen species, and extremely low emissions of particulates, have been demonstrated at such facilities as the Cool Water IGCC plant in California [8]. Third, IGCC plants produce fuel gas (also known as syngas) streams with concentrated hydrogen (H_2), as well as high levels of carbon monoxide (CO), which can be easily converted to CO_2. Capture of this CO_2 with high partial pressure prior to combustion requires the treatment of substantially smaller gas volumes than capture after combustion because the flue gas stream is not yet diluted with atmospheric N_2 and excess air. Hence, recovery of CO_2 in IGCC systems is potentially less expensive than in the conventional combustion systems.

Although IGCC technology presents the best environmental performance of all coal-based technologies [9], it is just in the beginning of its commercialization stage with only four commercial units operating in the world today (two in Europe and two in the U.S.). Currently, electricity generating cost, plant availability and operational performance of IGCC technology are not competitive with conventional coal power plants. Considering the environmental performance of IGCC technologies and growing interests in reducing atmospheric release of CO_2, I pose the following questions. How would the introduction of CO_2 mitigation policies affect the economic competitiveness of IGCC systems? Would IGCC, including CO_2 capture, become a feasible repowering option for existing coal-fired power plants?

The engineering-economic model presented here addresses these questions by characterizing the performance and cost of IGCC with CO_2 capture, the uncertainties associated with this technology, and its possible role in climate mitigation policies.

Process overview of IGCC system

A “traditional” IGCC system is composed of three main systems (gasification, clean-up and combined cycle power generation) and several auxiliary units (air separation, Claus unit for sulfur recovery, and waste water treatment). The degree of integration of these units leads to various configuration options. There are a number of gasification processes in commercial use or under development, including those produced by Texaco, Shell, E-Gas (formally Dow), BGC/Lurgi, and KRW. Texaco is considered the most prominent system because of the success of the Cool Water demonstration plant [10-11], and because it is the most widely used commercial gasifier (mainly in the petrochemical industry, using low-value feed stocks such as heavy oils and petroleum coke). Although ongoing research by the U.S. Department of Energy and others is focused on developing dry physical and chemical hot gas cleanup techniques to reduce the efficiency penalty associated with syngas cooling [12-13], the author have only considered technologies currently used at commercial plants or demonstration plants at commercial scale in this study. Therefore a typical design for an IGCC system uses a Texaco gasifier and cold gas cleanup processes that are representatives of the technologies employed in the Cool Water demonstration plant and in use elsewhere today. This reference IGCC plant without CO_2 capture is shown in figure 1.

In this reference plant, coal is fed to the gasifier in a water slurry form. Oxygen is used to combust only a portion of the coal in order to provide the thermal energy needed for endothermic gasification reactions. The carbon monoxide and hydrogen rich syngas from the gasifier is quenched and cooled down by various heat exchangers, providing some energy for the steam cycle. A gas scrubber is used to remove particulates, and an acid gas removal system is used for sulfur by-product recovery. Before syngas is fed into the combined cycle system for power generation, it is saturated to reduce NO_x formation in the gas turbine. The hot gas turbine exhaust passes through a Heat Recovery Steam Generator (HRSG) to provide energy to a steam turbine bottoming cycle. Power is generated by both the gas turbine and the steam turbine.

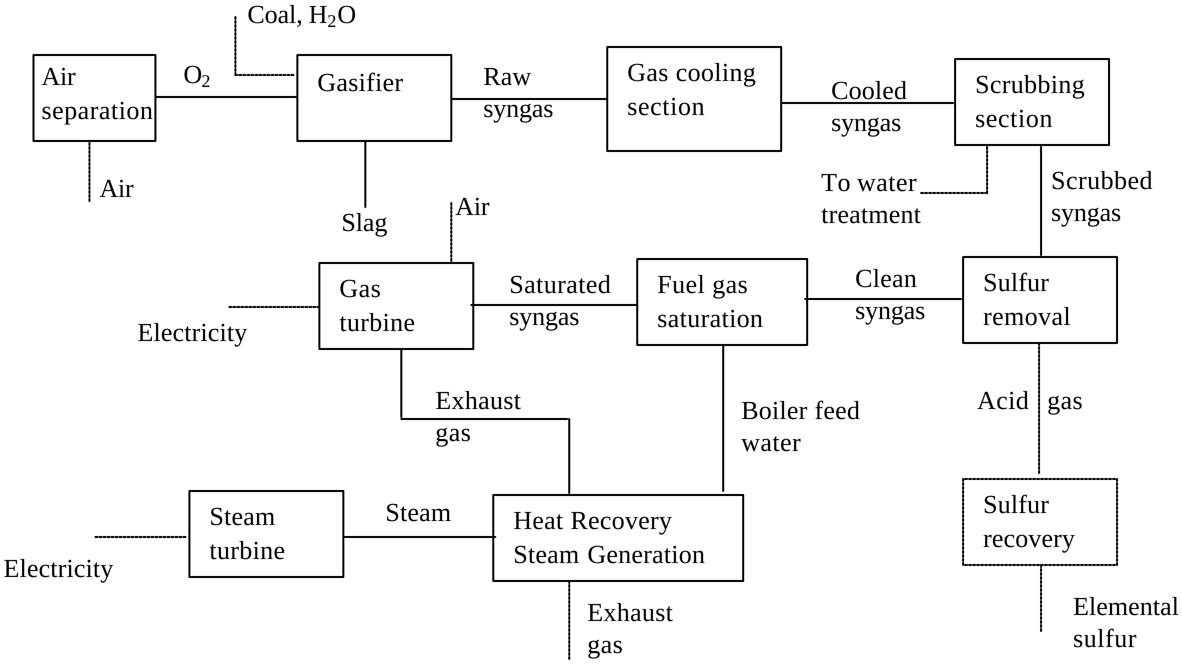

Figure 1. An O_2-blown, cold gas cleanup IGCC system process

IGCC with CO_2 capture

Compared to natural gas combined cycle (NGCC) and pulverized coal (PC) power plants using chemical absorption processes for CO_2 capture, IGCC systems have the advantage of using less energy-intensive physical absorption processes. Physical absorption using Selexol solvent is current the most effective technique for removing CO_2 from IGCC fuel gases [14-15]. In order to take advantage of the high gasification pressure for CO_2 physical absorption, two additional units are added, one is the Water Gas Shift (WGS) reaction unit, and the other one is the Selexol unit for CO_2 absorption. Most of the CO in the raw syngas is converted into CO_2 through WGS reaction. Then CO_2 is removed from the shifted syngas through a physical absorption unit. The CO_2 lean fuel gas (mainly H_2) is burned in a gas turbine for power generation. A typical IGCC system with Selexol-based CO_2 capture is illustrated in Figure 2.

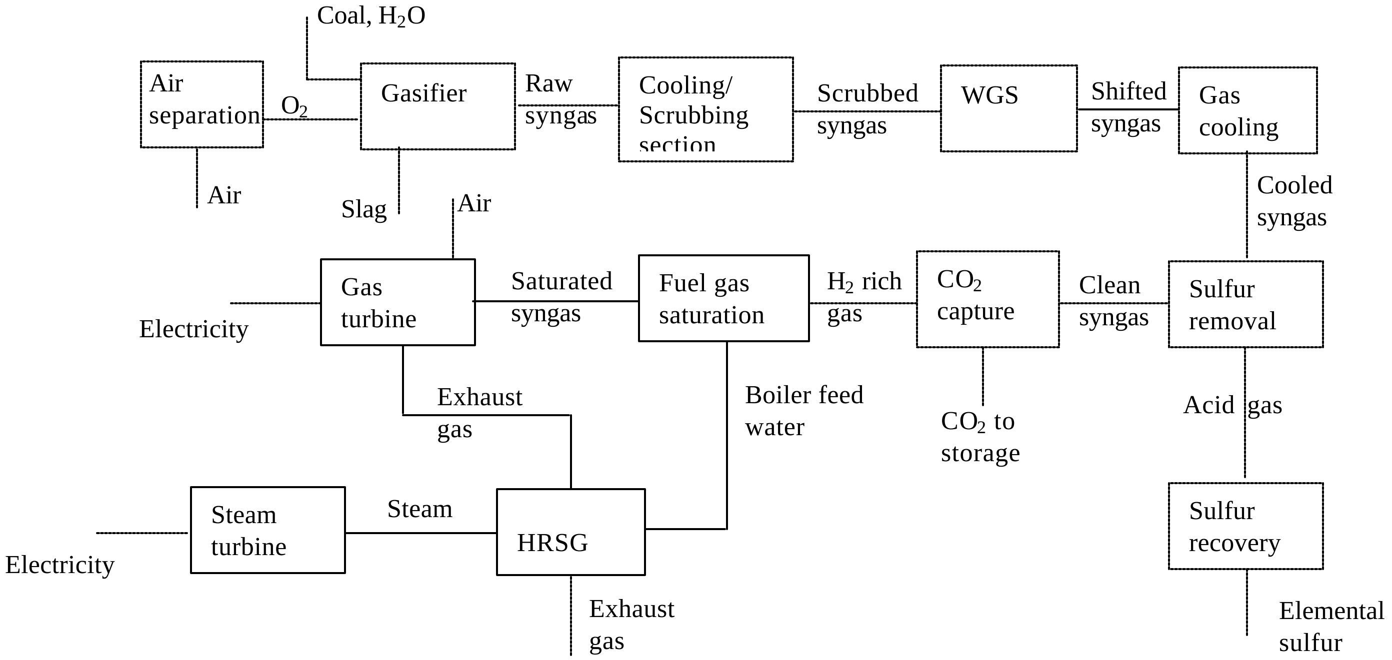

Figure 2. An IGCC system with Selexol-based CO_2 capture

The WGS reaction is well known and widely practiced throughout the chemical industry. It is a reversible and exothermic reaction, shown by Equation 1.

$$H_2O(g) + CO(g) \Leftrightarrow CO_2(g) + H_2(g) \qquad (\Delta H = -40.6 kJ/mol) \qquad \text{(Eq. 1)}$$

It is also an equilibrium controlled reaction, where the equilibrium constant K_{eq} depends on the reaction temperature (T in degrees Kelvin), shown by Equation 2 [16].

$$\ln(K_{eq}) = -13.19 + 5.54\times10^{-4} T + 1.12\times10^{-7} T^2 + 1.077\ln(T) + 5645.56/T - 49195/T^2 \qquad \text{(Eq. 2)}$$

Being exothermic, the reaction is favored by low temperatures. However, this low temperature decreases the speed of reaction. As illustrating in Figure 3, in practice, two WGS reactors are employed. Most of CO is consumed at the high temperature reactor with a fast reaction rate, but only partial conversion of CO to CO_2. A higher CO conversion rate is then achieved by adding a second lower temperature reactor. The reaction heat is recovered for use in the steam cycle and in fuel gas saturation.

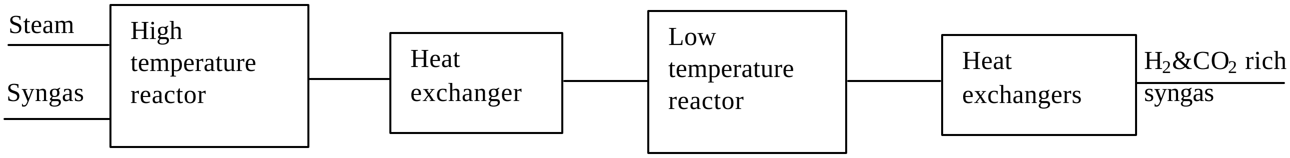

Figure 3. Water gas shift reaction process

Selexol is a commercially available physical solvent that is a mixture of dimethyl ether and polyethylene glycol [17]. It is a widely used physical absorption process for acid gases treatment, such as bulk CO_2 capture, because it is a non-corrosive, nontoxic, low viscosity liquid with low vapor pressure and a low heat of absorption [18]. The solvent quality of Selexol is maintained by keeping the water and oil contents at a nominal value, which is pretty simple [19].

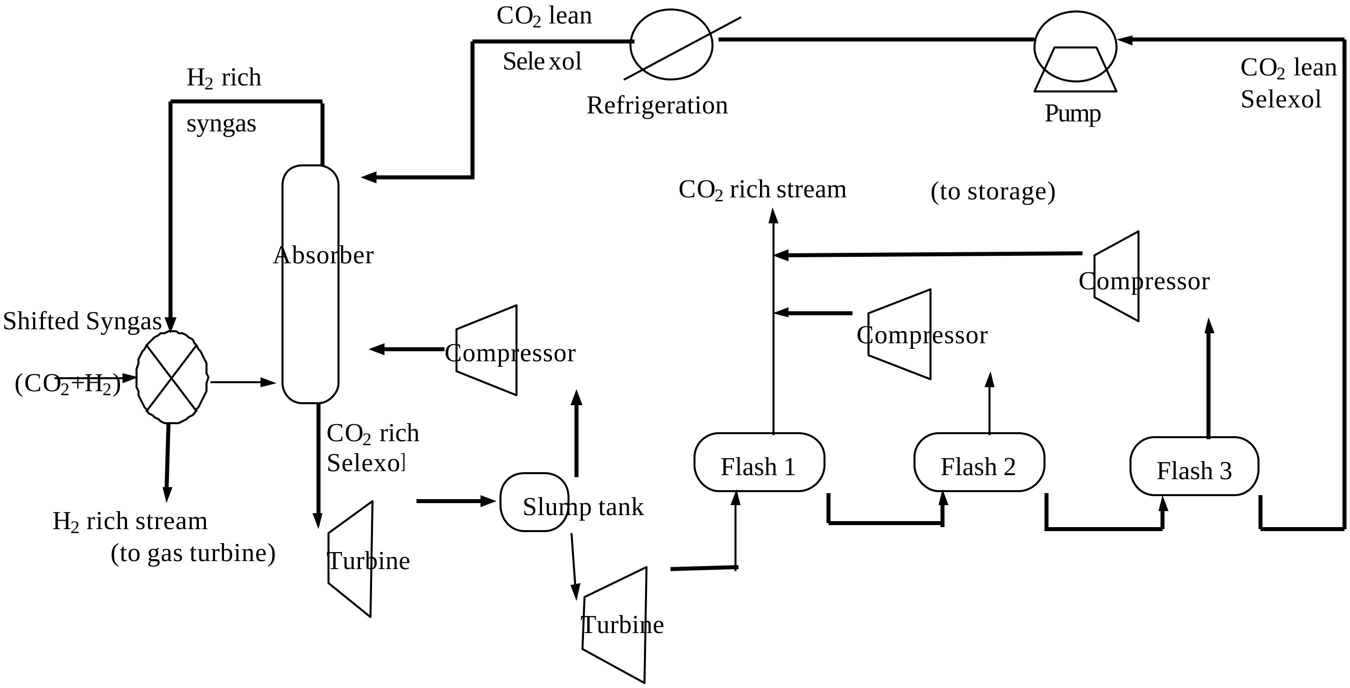

Figure 4. Selexol based CO_2 capture process

A general schematic of this Selexol process for CO_2 capture is given in Figure 4. CO_2 from the cooled, shifted syngas is absorbed by the CO_2 lean solvent at high pressure in a counter flow absorber. The pressure energy in the CO_2 rich solvent is recovered with one or two hydro turbines. Most of the H_2 entrained and absorbed in the solvent is released in the slump tank and recycled to the absorber. Most of the CO_2 absorbed by the solvent is recovered through flashing. The lean solvent is then compressed, cooled, and fed back into the absorber. There is no heat demand for solvent regeneration in the Selexol process because solvent recovery is possible through flashing. As a result the net power loss associated with the Selexol-based CO_2 capture is much less than other CO_2 recovery systems such as amine systems [20].

IGCC Model development

Performance and cost models of an IGCC system with CO_2 capture were developed based on a previously developed model of an IGCC system without CO_2 capture [21-22]. The original IGCC system model was modified in two ways. First, the original cost model was updated to reflect the progress of IGCC systems in recent years [9-10, 23-30]. Second, new performance and cost models of the WGS reaction system and the Selexol system were developed, and incorporated into the reference plant model to account for the effect of CO_2 capture on performance and cost.

WGS reaction system modeling and process integration

A general water gas shift reaction process performance model was developed in Aspen Plus (a detailed chemical process simulator). It includes a high temperature reactor, a low temperature reactor and several heat exchangers for heat recovery. Industrial experiences show that the reactions at the two reactors are close to equilibrium states. Hence, in this model, the reactions in the two reactors are assumed to achieve equilibrium states, and the approach temperature method is used to adjust the equilibrium temperatures to account for non-equilibrium conditions.

This process involves substantial cooling because of the exothermic shift reaction. The heat removed during cooling must be recovered and integrated into the system to minimize the energy penalty associated with CO_2 recovery [23]. As illustrated in Table 1, three recovery options have been investigated, and preliminary simulation results showed that the third one has the lowest energy penalty. Therefore, the third option has been selected as the heat recovery strategy.

Table 1: Heat recovery integration options

Option 1: Steam generation only	Option 2: Fuel gas preheating with supplemental steam generation	Option 3: Fuel gas saturation and preheating
All of the available energy is used to produce steam	Recovered energy is applied as far as possible for preheating the fuel gas stream to the gas turbine. Heat that cannot be used for fuel gas preheating is used in the HRSG	Moisture that has condensed out of the synthesis gas stream during the final cooling stage of the gas is injected into the fuel gas as it is heated by recovered heat.

The performance model for the WGS reactor system is represented by a series of equations developed to represent the relationship of output parameters (flow rate, temperature change, CO conversion, catalyst volume, reaction rate) to WGS input parameters (flow rate, temperature, pressure, syngas composition, steam/carbon ratio). These equations are based on the WGS reaction mechanism and employ regression analysis of the Aspen Plus output data. Independent variables included in the regression equations were selected based on engineering and chemical principles, and an analysis of the *t*-statistic for the coefficient associated with each independent variable. After this iterative approach to regression equation development, the goodness-of-fit of each equation was evaluated both graphically and using F-statistic. The input and output parameters of the performance model are given in Table 2.

Table 2. The input and output parameters of WGS performance model

Input parameter			Output parameter	
Syngas from gasifier	Temperature (F)		Shifted syngas	Temperature (F)
	Pressure (psia)			Pressure (psia)
	Flow rate (lb-mole/hr)			Flow rate (lb-mol/hr)
	Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4			Molar concentration CO, CO_2, H_2O, H_2, N_2, CH_4
Steam/carbon molar ratio			Reaction rate	Catalyst volume (ft^3)
Cold fuel gas& water	Temperature (F)		Heated fuel gas	Temperature (F)
	Pressure (psia)			Pressure (psia)
	Flow rate (lb-mol/hr)			Flow rate (lb-mol/hr)
	Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4			Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4
Feed water	Pressure (psia)		Saturation water & steam	Temperature (F)
	Temperature (F)			Flow rate (lb-mol/hr)

The total cost of the WGS system includes both capital and O&M components. The O&M cost includes labor, maintenance, and catalyst replacement. The capital cost of each unit is due primarily to the reaction vessels, heat exchangers, and initial catalyst, and has been evaluated based on the flow rate, pressure, temperature, and/or reaction rate, which come from the performance model. The details of the performance and cost model of the WGS reaction system used in this analysis are summarized in the Appendix A.

Performance and cost model of Selexol process

The first step in the performance simulation is to calculate the solvent flow rate. The solubility of CO_2 in the Selexol solvent is a function of partial pressure and temperature. In turn, the temperature also depends on the absorption heat from CO_2 capture and the heat transfer between solvent and syngas. Hence an iterative calculation is required to equilibrate the temperature change and the absorption amount of CO_2. The process for calculating the Selexol flow rate is represented in Figure 5.

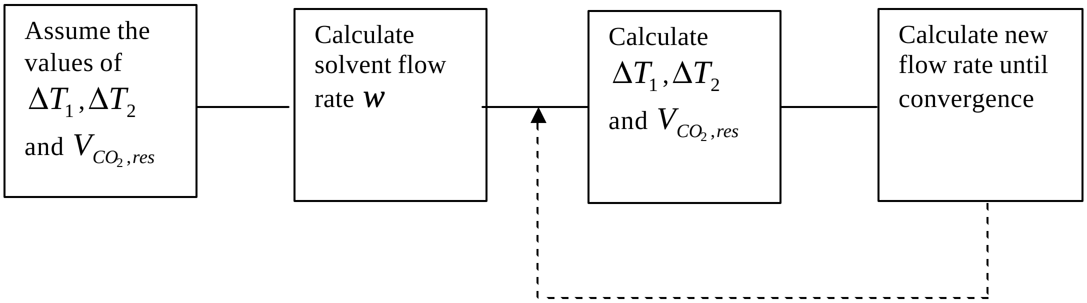

Figure 5. Iterative method for calculating the Selexol solvent flow rate (Here ΔT_1 is the solvent temperature increase caused by heat transfers; ΔT_2 is the temperature increase caused by the solution heats; $V_{CO_2,res}$ is the residual CO_2 in the lean solvent)

There is no net heat requirement in the Selexol process because the solvent is regenerated through pressure flashing. However, electrical power input is required to compress the recycling gas from the slump tank, the CO_2 lean solvent from the flash tank, and the CO_2 product. At the same time, some electricity can be generated through the power recovery hydro turbine. The total power consumption is the difference between the power input and the recovered power. In order to reduce the power consumption for CO_2 compression, three flashing tanks with different pressures are used to release the CO_2 captured by the Selexol. Pressure selection for each flashing tank is an optimization problem. However, sensitivity analysis showed that the power consumption for CO_2 separation and compression does not change appreciably when these pressures are varied. Therefore, the pressures have been chosen in accordance with common industrial practice. The input and output parameters of the performance model are given in Table 3. The capital cost of each unit in the Selexol process are based on the input and output parameters of performance model. Appendix B gives more details on this model development.

Table 3. Input and output parameters of Selexol model

Input parameter				Output parameter		
Syngas input	Flow rate (mole/s)	f_1		Fuel gas output	Flow rate (mole/s)	f_2
	Pressure	p_1			Pressure	p_2
	Temperature	T_1			Temperature	T_2
	Molar concentrations	$[CO]_1$			Molar concentrations	$[CO]_2$
		$[CO_2]_1$				$[CO_2]_2$
		$[H_2]_1$				$[H_2]_2$
		$[CH_4]_1$				$[CH_4]_2$
		$[H_2S]_1$				$[H_2S]_2$
		$[COS]_1$				$[COS]_2$
		$[NH_3]_1$				$[NH_3]_2$
		$[H_2O]_1$				$[H_2O]_2$
CO_2 removal percentage				CO_2 flow	Flow rate (mole/s)	f_5
					Pressure	P_5
				Refrig. power	Power recovery	Comp. power

Case study results

The models described above were employed to investigate two problems associated with CO_2 capture from IGCC systems: (1) CO_2 mitigation cost based on current IGCC technology; (2) the effects of uncertainties and variability associated with IGCC plant and the CO_2 capture systems.

Table 4 summarizes the operating conditions of the reference plant and plant with CO_2 capture used in this study. As discussed previous, gasifier type and operating conditions were chosen based on typical commercial equipment. Gas turbine inlet temperature and pressure ratio are representative of state-of-the-art, heavy-duty turbines. The three-pressure level reheat steam cycle conforms to the standard adopted for large combined cycle systems [24-25].

Table 4. Operating conditions of IGCC system

Plant size (net power output, MWe)	504.5
Capacity factor	0.75
Fuel	Illinois No.6 Coal
Gasification Section (Texaco quench)	
Gasification pressure (psia)	615
Gasification temperature (F)	2400
Heat loss in gasifier (% of input LHV)	0.5
Overall pressure losses along syngas path (psia)	150
Water/coal ratio in slurry	0.503
Gas Turbine Section (GE MS7001F)	

GT inlet temperature (F)	2410
Pressure ratio	15.5
Steam Section	
Pressure (psia)	1465/310/70
Superheated steam temperature (F)/reheat temperature (F)	993/993
CO_2 capture section (WGS+Selexol)	
Steam/Carbon ratio	2.5
Temperature of syngas inlet high temperature reactor (F)	500
Temperature of syngas inlet absorber (F)	100
Lean Selexol solvent temperature (F)	30
CO_2 capture percentage (%)	90
Pressure at flash tank 1 (psia)	60
Pressure at flash tank 2 (psia)	14.7
Pressure at flash tank 3 (psia)	5
Power recovery turbine efficiency (%)	77
Selexol pump efficiency (%)	78
Recycle gas compressor efficiency (%)	80
CO_2 compressor efficiency (%)	79
CO_2 product pressure (psia)	2100

The total capital requirement (TCR) of the IGCC system with and without CO_2 capture, and the overall cost of electricity (COE) are calculated following the EPRI cost estimating guidelines [31]. The assumptions used in this evaluation are summarized in Table 5. Detailed model outputs appear in Appendix C.

Table 5. Economic and financial assumptions of the IGCC plant

General facilities factor	15%PFC*	Cost year	2000
Engr&Home office Fee	10%PFC	Number of shifts	4.25
Project contingency	15%PFC	Average labor rate ($/hr)	19.7
Process contingency	Variables	Fuel price ($/MMBtu)	1.26
Sales tax	5%	CO_2 transport and storage ($/ton)	10
Interest rate	10%	Years of construction (yr)	4
Escalation rate	0	Lifetime (yr)	30

*Process facilities capital (PFC)—total construction cost of all on-site processing equipment including all direct and indirect construction costs, related sales taxes and shipping costs.

To estimate the cost per ton CO_2 avoided, the plants with carbon capture and storage (CCS) is assumed to use the same amount of fuel as the reference plant, while holding all else constant [32]. The cost of CO_2 avoided is then given by,

$$\$/ton\ \ CO_2 = \frac{(COE)_{capture} - (COE)_{ref.}}{(kg/kWh)_{ref} - (kg/kWh)_{capture}}$$

Table 6 compares the power output, thermal efficiency, capital cost, cost of electricity (COE), and CO_2 emissions of an IGCC plant with CO_2 capture to a reference plant without capture. With 90% CO_2 capture from shifted syngas and \$10/ton for captured CO_2 transportation and storage, the cost of CO_2 avoided is approximately \$29/ton CO_2. The CO_2 emission rate decreases from 1.83 lb/kWh to 0.25 lb/kWh, while the capital cost increases from 1285\$/kWh to 1759\$/kWh. The net power output decreases by 11.3% (from 505 MWe to 448 MWe). Figure 6 gives the breakdown of CO_2 mitigation cost. Transportation and storage of CO_2 accounts for about one third of the total mitigation cost, power required for the Selexol absorption process accounts for one fifth of the mitigation cost, and the capital costs of the Selexol and WGS processes accounts for 28% of the mitigation cost.

Table 6. Output of simulation results (detailed results given in Appendix C)

Item	Reference plant w/o capture	IGCC with CO_2 capture
Net output (MWe)	504.5	447.5
Gas turbine output (MWe)	388.2	370.9
Steam turbine output (MWe)	185.4	190.8
Efficiency (%, based on HHV)	36.8	32.7
CO_2 emission rate (lb/kWh)	1.828	0.251
Capital cost (\$/kW)	1285	1759
COE (mills/kWh)	39.7	60.3
CO_2 mitigation cost (\$/ton CO_2 avoided)	None	28.80

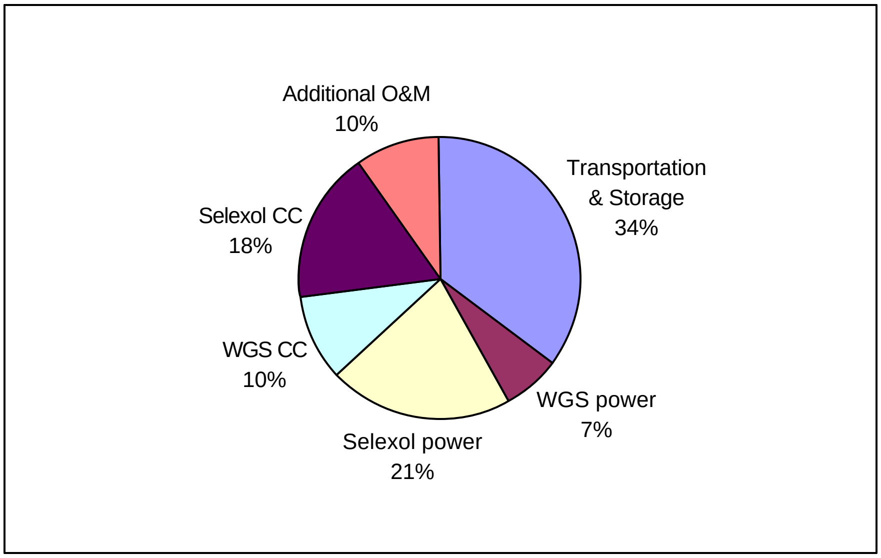

Figure 6. CO_2 mitigation cost breakdown

The effects of variability in capacity factor and fuel cost on the cost of CO_2 avoided are illustrated in Figure 7. The cost of CO_2 avoided is proportional to the price of coal, but the influence of coal price is not appreciable. For example, if the coal price is doubled, the cost of CO_2 avoided will only increase by 1.2 \$/ton CO_2. Compared with fuel price, plant utilization rate (capacity factor) plays a more important role in determining the cost of CO_2 avoided.

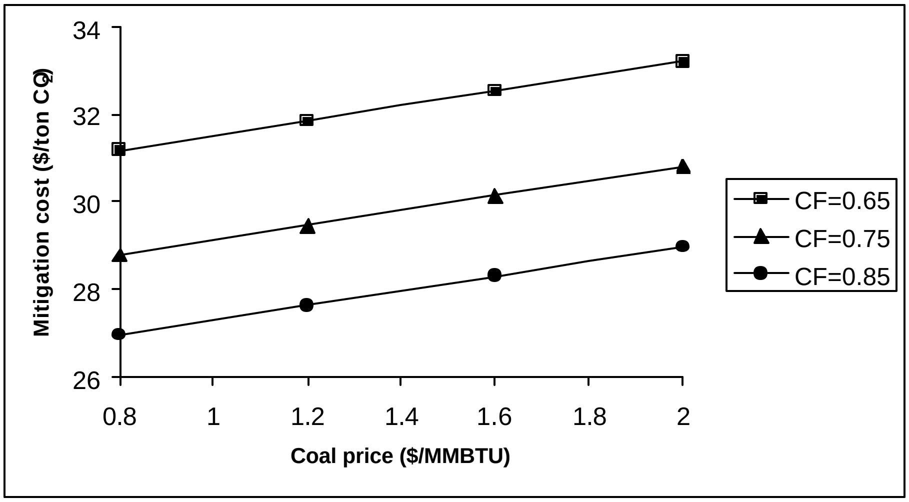

Figure 7. CO_2 mitigation cost vs. capacity factor and coal price

Uncertainty analysis

There is still limited large scale, commercial experience with IGCC and Selexol systems for CO_2 capture. Consequently, there is substantial uncertainty associated with using the limited performance and cost data available for these systems. Systematic analysis of uncertainties in evaluating the risks and potential pay-offs of this new process is needed. In this paper, the term uncertainty is used loosely to include variability (for example, in nominal process design values) as well as true uncertainty in the value of a particular parameter. To explicitly represent uncertainties in the performance and cost estimates for IGCC systems with Selexol-based CO_2 capture, a probabilistic modeling approach has been applied based on the detailed engineering and cost models discussed above. Probability distributions were assigned to performance and cost parameters of the IGCC, WGS reaction, and Selexol systems. The distributions represent the uncertainty in each parameter based on data analysis and literature review. The probability distributions for each input variable in a model are propagated through the model using Latin Hypercube sampling (LHS). The distribution functions assigned to the parameters of the CO_2 capture process and the IGCC system are listed in Table 7 and 8, respectively. The methodology for encoding uncertainties as probability distributions is explained in Appendix 4

Table 7. Distribution functions assigned to Selexol-based CO_2 capture process

Performance parameter	Unit	Nominal value	Distribution function
Steam/Carbon ratio		2.5	Triangle(2,2.5,3)
CO_2 removal efficiency	%	90	Triangular (85,90,97)
Approach temperature in high temperature reactor	F	25	Uniform(20,30)
Approach temperature in low temperature reactor	F	15	Uniform(10,20)
Pressure loss	%	0.5	Triangular(0.2,0.5,1)
Temperature of syngas fed into high temperature reactor	F	500	Triangular(450,500,550)
Mole weight of Selexol	lb/mole	280	Triangular(265,280,285)
Pressure at flash tank 1	Psia	60	Uniform(40,75)
Pressure at flash tank 2	Psia	20	Uniform(14.7,25)
Pressure at flash tank 3	Psia	7	Uniform(4,11)
Power recovery turbine efficiency	%	77	Triangular(72,77,85)
Selexol pump efficiency	%	78	Triangular(75,78,85)
Recycle gas compressor efficiency	%	80	Triangular(75,80,85)
CO_2 compressor efficiency	%	79	Triangular(75,79,85)
CO_2 product pressure	Psia	2100	Triangular(1100,2100,2400)
Refrigeration evaporation temperature	F	10	Triangular(-10,10,15)
Temperature factor of CO_2 solubility		0.09	Uniform(0.088,0.0936)
Cost parameter	**Unit**	**Value**	**Distribution function**
High temperature catalyst cost	\$/ft^3	50	Triangular(35,50,60)
Low temperature catalyst cost	\$/ft^3	250	Triangular(220,250,290)
Selexol solvent cost	\$/lb	1.96	Triangular(1.32,1.96,3)
Process contingency of WGS system	% of DC	5	Triangular(2,5,10)
Process contingency of Selexol system	% of DC	10	Triangular(5,10,20)
Maintenance cost of WGS system	% of TC	2	Triangular (1, 2, 5)
Maintenance cost of Selexol system	% of TC	5	Triangular(2,5,10)
CO_2 product pressure	Psia	2100	Triangle(1200, 2100, 3500)
CO_2 transportation and storage	\$/ton CO_2	10	Normal(10,3)

Table 8. Distribution functions assigned to IGCC system

Parameter	Unit	Deterministic value	Distribution function
Capital cost parameters			
Engineering and home office fee	% of TPC	10	Triangular(7,10,13)
Indirection construction cost factor	% of TPC	20	Triangular(15,20,20)
Project uncertainty	% of TPC	12.5	Uniform(10,15)
General facilities	% of TPC	20	Triangular(15,20,25)
Process contingency			
Oxidant feed	% of DC	5	Uniform(0,10)
Gasification	% of DC	10	Triangular(0,10,15)

Selexol	% of DC	10	Triangular(0,10,20)
Low temperature gas cleanup	% of DC	0	Triangular(-5,0,5)
Claus plant	% of DC	5	Triangular(0,5,10)
Beavon-Stretford	% of DC	10	Triangular(0,10,20)
Process condensate treatment	% of DC	30	Triangular(0,30,30)
Gas turbine	% of DC	12.5	Triangular(0,12.5,25)
Heat recovery steam generator	% of DC	2.5	Triangular(0,2.5,5)
Steam turbine	% of DC	2.5	Triangular(0,2.5,5)
General facilities	% of DC	5	Triangular(0,5,10)
Maintenance costs			
Gasification	% of TC	4.5	Triangular(3,4.5,6)
Selexol	% of TC	2	Triangular(1.5,2,4)
Low temperature gas cleanup	% of TC	3	Triangular(2,3,4)
Claus plant	% of TC	2	Triangular(1.5,2,2.5)
Boiler feed water	% of TC	2	Triangular (1.5, 2, 4)
Process condensate treatment	% of TC	2	Triangular(1.5,2,4)
Gas turbine	% of TC	1.5	Triangular(1.5,1.5,2.5)
Heat recovery steam generator	% of TC	2	Triangular (1.5, 2, 4)
Steam turbine	% of TC	2	Triangular(1.5,2,2.5)
Other fixed operating cost parameters			
Labor rate	$/hr	19.5	Uniform(17,22)
Variable operating cost parameters			
Ash disposal	$/ton	10	Triangular(10,10,25)
Sulfur byproduct	$/ton	75	Triangular(60,75,125)
Fuel cost	$/MMBtu	1.26	Triangular(1,1.26,1.41)
Land cost	$/kW	3	Triangular(1.6,3,4)

Several of the parameters in the above tables were found to be correlated or expected to be correlated. The probabilistic simulations were exercised both with and without considering parameter correlations to determine if model results are sensitive to parameter correlation. Simulations using parameter correlations produced only minor effect on the results. Therefore, for convenience, the following case study presents the results based on uncorrelated sampling.

Figure 8 shows the effect of considering the uncertainty and design variability in performance and cost parameters of CO_2 capture (WGS and Selexol process) on the cost of CO_2 avoided. CO_2 solubility contributes only slightly to the total uncertainty. The uncertainty in the performance model contributes about $3/ton CO_2 to the total mitigation cost uncertainty. Most of this is from uncertainty in the efficiency of turbo-machinery for the absorption process. The probabilistic simulation with the uncertainty from the performance and cost models results in a CO_2 avoided cost between $26 and $32/ton. Compared to the deterministic value of $29/ton, both the mean and median are $1/ton higher.

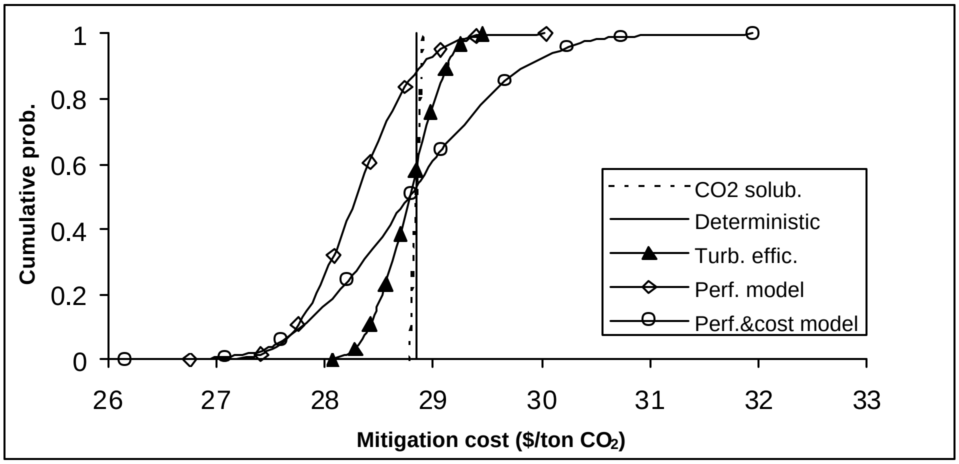

Figure 8. Effect of WGS and Selexol performance and cost uncertainty on the cost of CO_2 avoided (The simulations for this figure did not take into account the uncertainties in CO_2 product pressure and the cost of CO_2 transportation and storage)

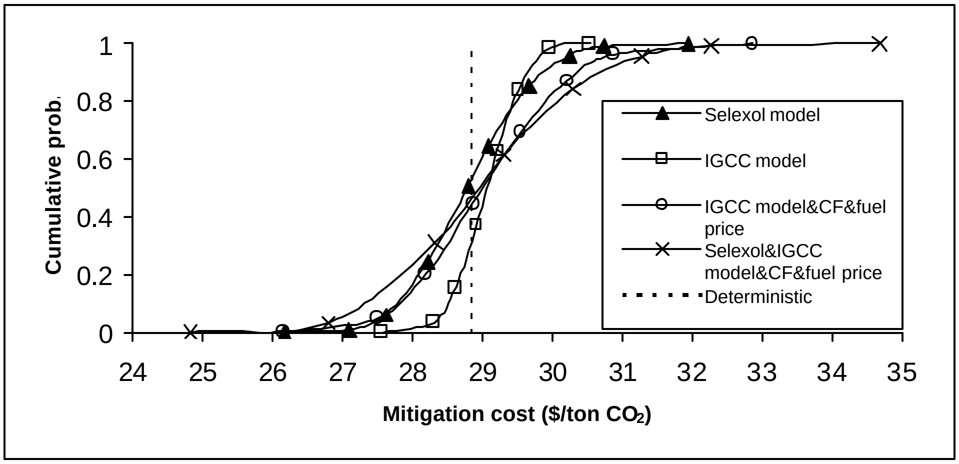

Figure 9. Effect of IGCC model, fuel price and capacity factor uncertainty on the cost of CO_2 avoided

The performance and cost of the reference IGCC plant can also affect the mitigation cost. Figure 9 shows the effect of the coupled uncertainties in CO_2 capture model (WGS and Selexol), IGCC plant model, fuel price and capacity factor. The cost of CO_2 avoided ranges from \$25 to \$35/ton, and the 90% probability interval ranges from \$27 to \$31/ton. There is a 58 percent probability that the mitigation cost would be higher than the deterministic estimation. This simulation also shows that mitigation cost is not very sensitive to the uncertainties in the capital cost of IGCC plant.

The final CO_2 product pressure and disposal cost (including transportation and storage cost) are highly site specific. As illustrated in Figure 10, if the uncertainties associated with these two aspects are taken into account with all the other uncertainties, the mitigation cost is found to have a much wider range, from \$10 to \$46/ton, and the 90% confidence interval is from \$23 to \$35.5/ton. This figure also shows that the mitigation cost is much more sensitive to the storage cost than to the final CO_2 pressure.

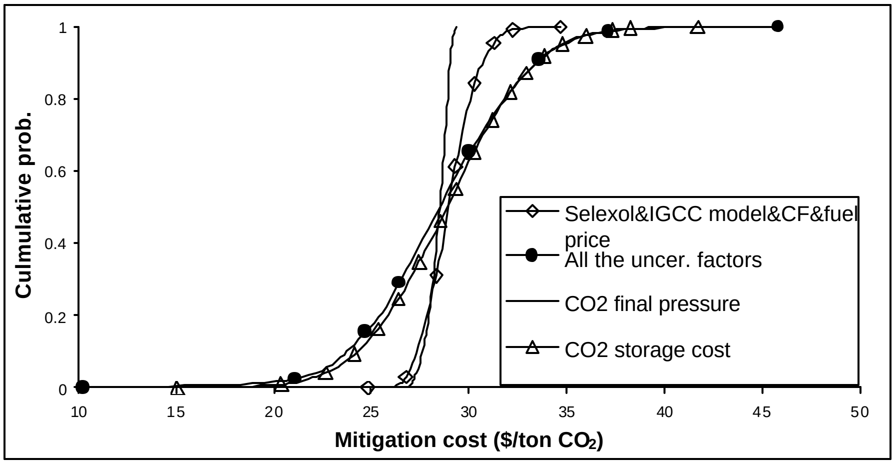

Figure 10. Total effect of uncertainty on the cost of CO_2 avoided

IGCC repowering with CO_2 capture

North America has over 320,000 MWe of existing coal-based power plants, which accounts for 35% of the total installed capacity and 45% of the total annual power generation in North America [33-34]. Most of the existing coal-based power plant capacities are pulverized coal (PC) boilers that are 25-35 years old. These existing coal-based power plants have the highest CO_2 emission rate, due to the use of high carbon fuel (coal) and a relatively low thermal efficiency. What is the technical and economic potential to reduce CO_2 emissions from these existing power plants in the event that new environmental regulations place limits on carbon emissions? One recent study looked at retrofitting plants with an amine scrubber, and found this to be a costly measure that would substantially degraded plant performance [35]. IGCC repowering with CO_2 capture offers a substantially different option to this problem.

IGCC repowering can be defined as the integration of gasification units, gas turbine generator units and heat recovery units into an existing steam power plant. Compared to other repowering technologies, IGCC repowering without CO_2 capture is usually considered to be less attractive due to the expense of the gasification units [36], however, it does present several advantages. IGCC repowering can substantial increase the capacity and thermal efficiency of a plant. The net output of a repowered IGCC plant can be up to three times of the original steam cycle plant. At the same time, the environmental emissions of NOx, SOx, Hg and solid waste can be dramatically reduced [37-38]. Shorter construction time and re-use of existing equipment (cooling system, steam turbine/generator units), infrastructure (road/railroad connections, office building), and existing transmission capacity will reduce the capital cost relative to a new IGCC plant. Furthermore, re-use the existing plant land can simplify the complicated site studies and authorization procedures [39-40].

If the purpose of repowering is to mitigate CO_2 emissions, IGCC repowering can reduce CO_2 emissions while also improving capacity and efficiency, which other retrofitting options such as amine scrubbing, will not do. The rest of this paper analyzes this option in more detail.

Analysis of repowering options

There are three approaches for IGCC repowering: feedwater heating repowering, boiler hot windbox repowering and heat recovery repowering [41-42]. Feedwater heating repowering uses the gas turbine exhaust to heat the boiler feedwater. Windbox repowering utilizes the gas turbine exhaust as the combustion air for the existing boiler. Heat recovery repowering uses the gas turbine exhaust to generate steam in a Heat Recovery Steam Generator (HRSG), which replaces the existing boiler. In the first two approaches, the existing boilers have to be kept, and it is necessary to control CO_2 emissions from the existing boilers as well as from the gasifier. Therefore, these two approaches do not fully take advantage of the low CO_2 capture cost of the gasification process. Hence, for the goal of CO_2 capture, only the heat recovery repowering approach is an attractive choice for IGCC repowering with CO_2 capture.

Because gas turbines are only available in discrete sizes, the capacity of the gas turbines and steam turbine should match well to fully utilize waste heat from the gasification units and gas turbine. There is a range of steam turbine power output that that can be repowered with a given gas turbine. The range depends on the temperature and flow rate of gas turbine exhaust, throttle pressure and loading limitation of the existing steam turbine, and the heat recovery process employed. The lower boundary of the range is achieved under the most restrictive condition---the replacement of a non-reheat boiler by a gasifier, gas turbine, and HRSG with no modification to the either the steam turbine or the feedwater heating system. This configuration is illustrated in Figure 11. The maximum power output is achieved under the most ideal condition---the existing steam turbine has sufficient design margins so that it can incorporate a two pressure HRSG without a feedwater heating system, as shown in Figure 12.

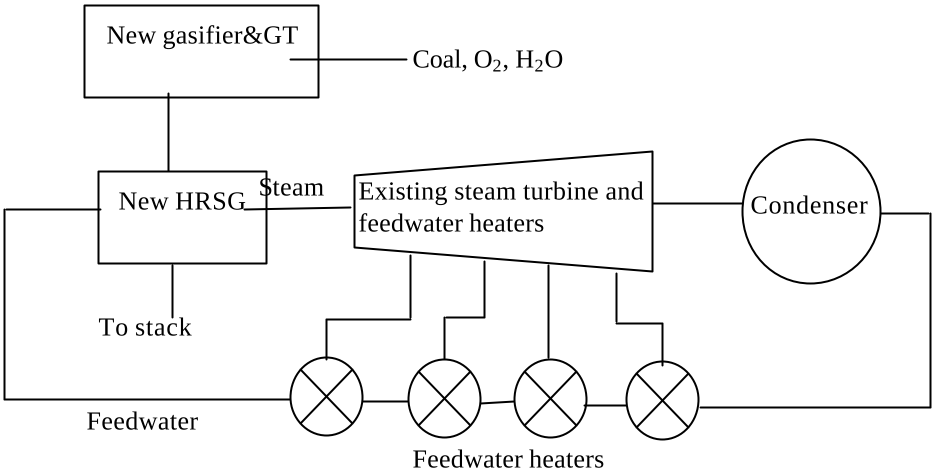

Figure 11. IGCC repowering with all feedwater heaters (minimum repowering case)

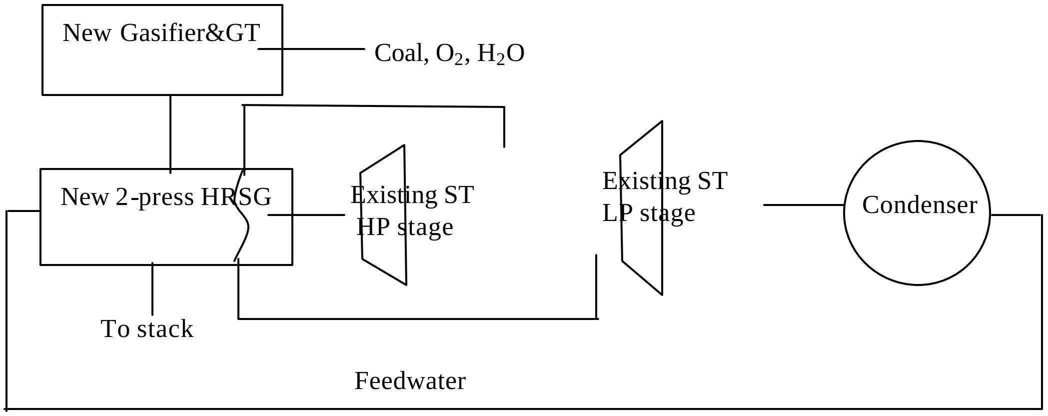

Figure 12. IGCC repowering without feedwater heaters (maximum repowering case)

A modified version of the performance and cost models described earlier was used to study the two repowering options. For the cost analysis all existing capital equipment is assumed to be fully amortized. If a Texaco quench gasifier with CO_2 capture and a GE MS7001F gas turbine operating at the conditions given in Table 4 are employed to repower a steam turbine operating at 1465 psig throttle conditions, through steam turbine performance estimation, a 69 MW steam turbine can be repowered for the minimum case, and a 91 MW steam turbine can be repowered for the maximum case. The performances of the two repowering alternatives are compared to a greenfield IGCC power plant in Table 9.

As shown in Table 9, compared to the greenfield IGCC plant, the installed cost of the repowering cases is reduced by 153$/kW and 271$/kW, respectively, for the two cases. The thermal efficiency and net output of the maximum repowering case is similar to that of the greenfield plant, whereas the thermal efficiency of the minimum repowering case is lower by 3.6 percentage points due to its relatively lower steam cycle efficiency. The COE of the maximum repowering case is 3.68 mills/kWh lower than the greenfield plant, while the minimum repowering case is 1.78 mills/kWh higher.

Table 9. Performance of greenfield and repowering IGCC plants with CO_2 capture (CF=0.75)

Case	Greenfield IGCC plant	Repowering plant, minimum case	Repowering plant, maximum case
Gas turbine capacity MW	185.5	184.2	184.2
Steam turbine capacity MW	95.0	69.4	91.4
Net output MW	222.8	197.6	218.9
Thermal efficiency (% as HHV)	32.5	28.9	32.0
CO_2 emission lb/kWh	0.25	0.29	0.26
TCR (Million dollars)	405	329	339
Installed cost $/kW	1818	1665	1547
COE (mills/kWh)	61.45	63.23	57.76
CO_2 avoidance cost (Based on greenfield plant w/o CO_2 capture)	30.1	33.4	24.9

Figure 13 compares the costs of electricity from repowered IGCC plants to those of plants retrofitted using amine based (MEA) CO_2 capture process [35]. The case of maximum IGCC repowering with CO_2 capture is the lowest cost system. Under some situations, even the minimum IGCC repowering case has better economic performance than retrofitting amine systems for CO_2 capture. In all cases, the cost of CO_2 avoided with IGCC is about half that for a conventional PC plant with an amine scrubber.

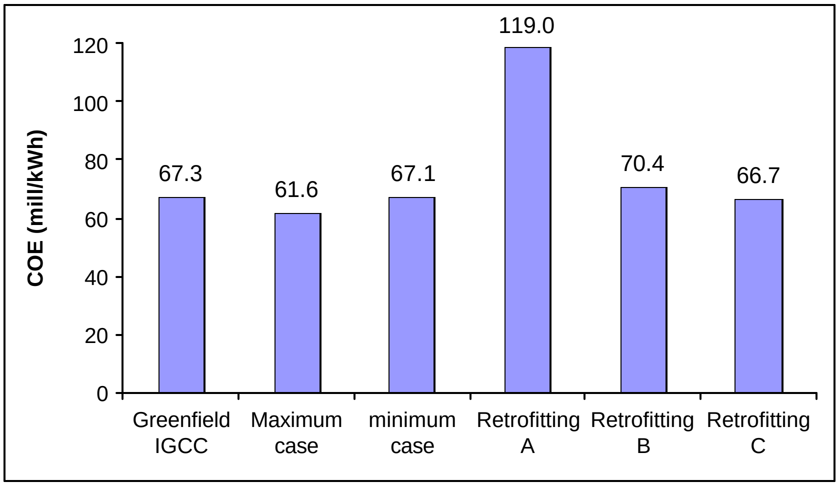

Figure 13. The comparison of COE of repowered plants and amine based retrofitted plants with CO_2 capture (Case A and B are for a plant burning low-sulfur coal with no other SO_2 emission controls. For case A, the plant is retrofitted with an MEA system. For case B, the plant is retrofitted with MEA plus a new FGD system. In case C, the low-sulfur coal plant has been already equipped with an FGD system for sulfur emission control, and it is retrofitted with an MEA system. In this comparison, my model input parameters were adjusted to make the comparison based on identical assumptions, so the COEs of IGCC plants in this figure are different from those in Table 9)

Additional considerations about IGCC repowering with CO_2 capture

To fully evaluate the application of using IGCC repowering with CO_2 capture in an existing facility, there are a number of additional factors that need to be considered.

- Available space: Reusing old sites is one of advantages of repowering, but IGCC repowering with CO_2 capture needs more equipment than other repowering approaches. Hence, site space could be at a premium for some locations, and installation costs may be increased due to space constraints and more complicated layouts. Such additional costs are not included in the current analysis.

- Heat rejection capability: Although the heat rejection from the steam turbine cycle is almost the same before and after the repowering, the low-energy, non-recyclable waste heat from the air separation unit and gasification process increases the total amount of heat rejection. In some cases this could exceed the heat rejection limitation permitted for a plant where condenser cooling is provided from a river, ponder or estuary. The total heat that may be rejected may be limited for environmental reasons. In this case, additional cooling towers may be required.

- Transmission constraint on bulk transmission system: IGCC repowering can triple the capacity of an existing plant and the total capacity of the repowered plant may surpass the capacity of the original transmission system. In such cases the transmission constraint will also have to be considered.

- The economical and technical issues discussed above are not the only factors that may influence the feasibility of implementing IGCC repowering with CO_2 capture. For instance, this option may be considered to be feasible even if it is economically marginal because in addition to reducing emissions, it may also reduce or eliminate the difficult process of siting and permitting new plants. It also allows society and utilities to gain IGCC construction, operating, and technology experience and knowledge necessary for successfully introducing the next generation of greenfield IGCC plants with carbon capture and sequestration.

Conclusion

This study developed a framework to analyze the effects of Selexol-based CO_2 capture on the performance and cost of an IGCC power plant. The analysis shows that based on commercially available technology, an appropriate integration of shift reactors and physical absorption system into an IGCC plant can reduce CO_2 emissions by approximately 90 percent. The cost of CO_2 avoided is half that for a conventional combustion plant with a chemical absorption process. The low cost of CO_2 avoided from

IGCC systems is significant and encourages future development and application of this system as a clean coal technology.

The uncertainties and variability in IGCC system designs with CO_2 capture come from the limited experience in producing, constructing and operating IGCC power plants with CO_2 capture. This study investigated the influence of uncertainties and variability associated with plant and process design on the cost of CO_2 avoided. CO_2 mitigation costs depend on assumptions about the plant and process design, but for IGCC systems, the uncertainty associated with CO_2 transport and storage has the largest impact on the cost of CO_2 avoided.

IGCC repowering with CO_2 capture may be an economically attractive option for existing steam power units. Compared to building greenfield IGCC plants, IGCC repowering is less capital intensive and has a shorter construction period. Hence it also provides an option for introducing new power generation technology with lower risk to utilities. The cost and feasibility of repowering is very site specific. This research identified a number of technical and non-technical factors and criteria that could apply. Under suitable conditions, IGCC repowering was shown to be a more cost-effective and attractive option for reducing CO_2 emissions from existing coal-fired plants compared to the alternative of retrofitting a CO_2 scrubber. Net increases in plant capacity and efficiency rather than decreases in both, are another benefit of this option. Since they reduce environmental impacts across the entire fuel cycle, further research is needed to identify the most promising applications of IGCC repowering based on detailed site-specific assessments.

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Appendix A

Performance and Cost Model of Water Gas Shift Reaction System

1. Introduction

The water gas shift reaction is widely used to produce hydrogen from carbon oxide and water steam. The reaction is given by [1].

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad -40.6 \text{ kJ/mol}$$

This reaction is a catalyst-aided reaction. There are two common commercially available catalysts. One is iron-based high temperature catalyst; the other is copper-based low temperature catalyst. The iron-based high temperature catalyst is effective in the temperature range from 650 to 1100F. The copper-based catalyst is effective in the temperature range from 450 to 650 F [2].

A general water gas shift reaction process model is developed in Aspen Plus, which is illustrated in Figure 1. It includes a high temperature reactor and a low temperature reactor and several heat exchangers for heat recovery. In this model, the syngas from a gasifier is mixed with steam at a given temperature and pressure, and then fed into the high temperature reactor. Most of the CO in the syngas is converted in the high temperature reactor at fast reaction rate. Further CO conversion is achieved in the low temperature reactor, but the syngas from the high temperature reactors has to be cooled before it's fed into the low temperature reactor because the water gas shift reaction is exothermic. The shifted syngas from the low temperature shift reactor is cooled down to 100F for CO_2 capture in a SELEXOL process. Part of the heat is used to heat the fuel gases from SELEXOL process, and the residual heat is recovered to heat the feed water of the steam cycle. In this model, the reactions in the two reactors are assumed to achieve the equilibrium states and the approach temperature method is used to adjust the equilibrium temperatures.

This Aspen model had been run thousands of times with different inlet temperatures, pressures and syngas compositions. Based on the simulation results, regression methods are used to look for the relationships between the inlet conditions and the final products of the water gas shift reaction, the energy consumption, and the makeup water amounts. Using these regression relationships, the whole water gas shift reaction system can be treated as a black box as following:

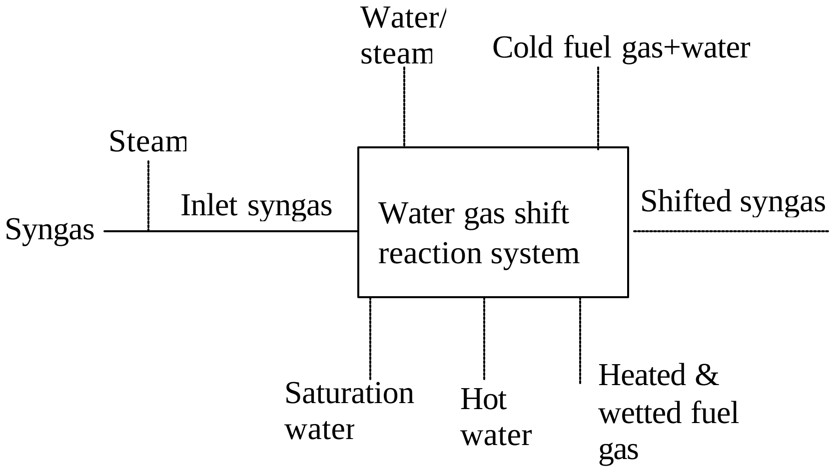

Figure 1. Mass and energy flow of water gas shift reaction system

2. Input and output parameters of the WGS performance model

The input and output parameters of this black box performance model are given in Table 1.

Table 1. The input & output parameters of WGS cost model

Input parameter			Output parameter	
Syngas from gasifier	Temperature (F)		Shifted syngas	Temperature (F)
	Pressure (psia)			Pressure (psia)
	Flow rate (lb-mole/hr)			Flow rate (lb-mol/hr)
	Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4			Molar concentration CO, CO_2, H_2O, H_2, N_2, CH_4
Steam/carbon molar ratio			Reaction rate	Catalyst volume (ft^3)
Cold fuel gas& water	Temperature (F)		Heated fuel gas	Temperature (F)
	Pressure (psia)			Pressure (psia)
	Flow rate (lb-mol/hr)			Flow rate (lb-mol/hr)

	Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4			Molar concentrations of CO, CO_2, H_2O, H_2, N_2, CH_4
Feed water	Pressure (psia)		Saturation water & steam	Temperature (F)
	Temperature (F)			Flow rate (lb-mol/hr)

2. Performance output

This section discusses the performance outputs of this model.

2.1 Shifted syngas composition

The water gas shifted reaction occurring at the high and low temperature reactors changed the concentrations of species and the temperature of the syngas. In order to represent the changes of concentrations, CO conversion is defined here as following,

$$CO \quad conversion(x) = \frac{CO \quad flowrate \quad in(lb \cdot mol/hr) - CO \quad flowrate \quad out(lb \cdot mol/hr)}{CO \quad flowrate \quad in(lb \cdot mol/hr)}$$

According to the definition of chemical equilibrium const, the CO conversion at the high temperature reactor is obtained and given by

$$x_1 = \frac{u_1 - \sqrt{u_1^2 - 4w_1v_1}}{2w_1}$$

where $u_1 = K_1([CO]_0 + [H_2O]_0) + ([CO_2]_0 + [H_2]_0)$

$$v_1 = K_1([CO]_0[H_2O]_0) - ([CO_2]_0[H_2]_0)$$

$$w_1 = K_1 - 1$$

$$K_1 = \exp(\frac{8240}{T_1 + dT_h + 459.67} - 4.33)$$

The total CO conversion in the two reactors is given by

$$x_{tot} = \frac{u_2 - \sqrt{u_2^2 - 4w_2v_2}}{2w_2}$$

$$u_2 = K_2([CO]_0 + [H_2O]_0) + ([CO_2]_0 + [H_2]_0)$$

$$v_2 = K_2([CO]_0[H_2O]_0) - ([CO_2]_0[H_2]_0)$$

$$w_2 = K_2 - 1$$

$$K_2 = \exp(\frac{8240}{T_2 + dT_l + 459.67} - 4.33)$$

Where T_1 and T_2 are the reaction equilibrium temperatures at the high and low temperature reactors, respectively. The two temperatures can be calculated using the following regression equations.

$$T_1(F) = 0.0122P_0 + 0.8668T_0 + 3297.049[CO_2]_0 - 21.634[H_2O]_0 + 356.234[H2]_0 + 401.392[N2]_0 + 2290.608[CO]_0[H_2O]_0$$

$$T_2(F) = -0.00136P_0 + 0.1031T_0 + 16608.87[CO_2]_0 + 404.098[H_2O]_0 + 331.976[H_2]_0 + 258.772[N_2]_0 - 1198.036[CO]_0[H_2O]_0 - 2105.116[CO_2]_0[H_2]_0$$

dT_h and dT_l are the approach temperatures for the high and low temperature reactors, respectively.

Flow rate of syngas and steam is $f_0(\frac{lb \cdot mol}{hr})$;

$T_0(F)$ is the temperature of syngas fed into the high temperature reactor;

Flow pressure is $p_0(psia)$.

$[I]_0$ is the molar fraction of syngas composition I before fed into high temperature reactor, here I is CO, H_2O, CO_2, H_2, N_2, and CH_4 etc.

Using the CO conversion in high temperature reactor, the CO concentration of syngas after the high temperature reactor is be given by,

$[CO]_1 = [CO]_0 \cdot (1 - x_1)$

Then the concentrations of H_2, CO_2 and H_2O after the low temperature reactor are given by,

$[H_2]_1 = [H_2]_0 + [CO]_0 \cdot x_1$

$[CO_2]_1 = [CO_2]_0 + [CO]_0 \cdot x_1$

$[H_2O]_1 = [H_2O]_0 - [CO]_0 \cdot x_1$

The concentrations of N_2 and CH_4 are not changed.

Using the two CO conversions given above, the CO concentration of shifted syngas after the low temperature reactor is be given by,

$[CO]_2 = [CO]_0 \cdot (1 - x_{tot})$

Then the concentrations of H_2, CO_2 and H_2O after the low temperature reactor are given by,

$[H_2]_2 = [H_2]_0 + [CO]_0 \cdot x_{tot}$

$[CO_2]_2 = [CO_2]_0 + [CO]_0 \cdot x_{tot}$

$[H_2O]_2 = [H_2O]_0 + [CO]_0 \cdot x_{tot}$

The concentrations of N_2 and CH_4 are not changed.

Where $[I]_2$ is the molar fraction of syngas composition I after the low temperature reactor, here I is CO, H_2O, CO_2, H_2, N_2, and CH_4 etc.

The CO conversion in the low temperature reactor is given by

$$x_2 = 1 - \frac{1 - x_{total}}{1 - x_1}$$

2.2 Flow rate of saturation water

The saturation water for the steam cycle is generated when the syngas from the high temperature reactor is cooled down to 450 F.

The temperature of saturation water is determined by the pressure of the stem cycle. According to the data in ASME 1967 steam and water table [4], the temperature is given by

$$T_{w,sat}(F) = 328.34 + 0.3565 p_{sc} - 0.0002 p_{sc}^2 + 6 \cdot 10^{-8} p_{sc}^3 - 7 \cdot 10^{-12} p_{sc}^4$$

where p_{sc} (psi) is the pressure of steam cycle (300~3000psi)

The heat released by syngas is given by,

$$Q_1(Btu/hr) = q_1 \cdot f_0$$

where $$q_1(Btu/lbmol) = p_0^{0.035972764} T_0^{1.2874051} [CO]_0^{1.143473372} [CO_2]_0^{-0.473384669} [H_2O]_0^{0.31497888} [H_2]_0^{0.000309005} [N_2]_0^{0.013926611}$$

Based on the total heat available and the saturation temperature, the flow rate of saturation water can be calculated.

2.3 Flow rate and temperature of the preheated feed water of the steam cycle

The syngas from the low temperature reactor is cooled down first by heating and wetting the fuel gas from SELEXOL up to 400 F, then it is further cooled down to 100F by preheating the feed water of the steam cycle.

The heat energy required to heat and wet the fuel gas from Selexol up to 400 F is given by,

$$Q_2(Btu/hr) = q_2 \cdot f_{fuel}$$

where

$$q_2(Btu/lbmol) = -0.13289 p_{fuel} - 11.2902 T_{fuel} + 3160.863[H_2]_{fuel} + 3225.942[N_2]_{fuel} + 3325.05[CO]_{fuel} + 3931.626[CO_2]_{fuel} + 22911.65[H_2O]_{fuel} + 4003.149[CH_4]_{fuel}$$

p_{fuel} (atm) is the pressure of fuel gas.

T_{fuel} (F) is the initial temperature of fuel gas.

f_{fuel} (lbmol/hr) is the flow rate of the fuel gas (including the added water. For wetting the fuel gas, users can determine how much water should be added. The default value of the cold water molar flow rate is one third of the molar flow rate of the fuel gas before adding water).

$[i]_{fuel}$ is the molar concentration of species i in the fuel gas (after adding water).

Then syngas outlet temperature of heat exchanger 2 is given by,

$$T_{h2,o} = 0.265509 \cdot T_2 + 0.090711\, p_2 - 0.02349 \frac{Q_2}{f_0} + 121.9409 \cdot [H_2]_2 + 454.8101 \cdot [H_2O]_2 + 125.5044 \cdot [CO_2]_2$$
$$+ 146.0441 \cdot [CO]_2 + 74.79687 \cdot [N_2]_2 + 95.8699 \cdot [CH_4]_2$$

The total heat released when syngas from low temperature is cooled down to 100 F is given by,

$$Q_{tot}(Btu/hr) = f_0(9.254524 \cdot T_2 - 0.31613 \cdot p_2 - 1386.1 \cdot [CO]_2 - 297.779 \cdot [CO_2]_2 - 1485.34 \cdot [H_2]_2$$
$$+ 17595.87 \cdot [H_2O]_2 - 1439.29 \cdot [N_2]_2 - 331.533 \cdot [CH_4]_2)$$

Then the heat used to preheat the feed water is given by,

$$Q_3 = Q_{tot} - Q_2$$

The inlet temperature of the feed water is assumed to be 57 F, its outlet temperature ($T_{c3,o}$) is determined to keep the log mean temperature difference of heat exchanger 3 at 40 F. Hence, it is given by,

$$\frac{(100-57)-(T_{h2,o}-T_{c3,o})}{\ln \dfrac{100-57}{T_{h2,o}-T_{c3,0}}} = 40$$

The heat needed to heat one lb-mole feed water from 57 F to $T_{c3,o}$ is given by,

$$q_3 (BTU / lb \cdot mol) = -1207 + 18.16115 \cdot T_{c3,o} - 0.04328 \cdot p_{sc}$$

$$(p_{sc} : 300 \sim 3000 psi; \quad T_{c3,o} \leq 400F)$$

Then the flow rate of the preheated feed water is

$$f_3 (lb \cdot mol / hr) = \frac{Q_3}{q_3}$$

3. Cost model of WGS process

The cost outputs of this model include total plant cost, total plant investment, total capital requirement, operation and maintenance cost.

3.1. Total Plant Cost (TPC)

The total plant cost is the sum of the process facilities capital (PFC), general facilities capital (GFC), engineering and home office fee, and contingencies including project contingency and process contingency.

3.1.1 The PFC for this water gas shift reaction system includes:

The costs of shift reactors are estimated based on the volumes of the reactor, which is 1.2 times of catalyst volumes [3]. The volumes of catalysts can be calculated as the following steps.

The space velocity (SV, 1/hr) is the ratio of the volumetric flow rate gas (VF) over the catalyst volume, so the catalyst volume can be given by,

$$V = \frac{f}{SV}$$

The space velocity is related to the fraction conversion (x) and the reaction rate by the following equation,

$$SV^{-1} = \int_0^x \frac{dx}{r}$$

The reaction rate can be given by

$$r = k\left[([CO]_{ini} - x)([H_2O]_{ini} - x) - \frac{([CO_2]_{ini} + x)([H_2]_{ini} + x)}{K}\right]$$

where k is the reaction rate constant; $[CO]_{ini}$, $[H_2O]_{ini}$, $[CO_2]_{ini}$, $[H_2]_{ini}$ are the inlet molar concentration of CO, H_2O, CO_2 and H_2, respectively; K is the equilibrium constant.

Then we can get the following equation,

$$\frac{k}{SV} = \frac{2K}{\sqrt{q}}\left\{\ln[\frac{2wx - u - \sqrt{q}}{2wx - u + \sqrt{q}} - \ln[\frac{-u - \sqrt{q}}{-u + \sqrt{q}}]\right\}$$

where $w = K - 1$

$$\sqrt{q} = \sqrt{u^2 - 4wv}$$

$$u = K([CO]_{ini} + [H_2O]_{ini}) + ([CO_2]_{ini} + [H_2]_{ini})$$

$$v = K([CO]_{ini}[H_2O]_{ini}) - ([CO_2]_{ini}[H_2]_{ini})$$

Using the above equations, the volume of high temperature catalyst is given by

$$V_1(ft^3) = \frac{VF_1}{SV_1}$$

where

$$\frac{k_1}{SV_1} = \frac{K_{1,real}}{\sqrt{q_1}}\left\{\ln[\frac{2w_1x_1 - u_1 - \sqrt{q_1}}{2w_1x_1 - u_1 + \sqrt{q_1}} - \ln[\frac{-u_1 - \sqrt{q_1}}{-u_1 + \sqrt{q_1}}]\right\}$$

where $w_1 = K_{1,real} - 1$

$$\sqrt{q_1} = \sqrt{u_1{}^2 - 4w_1v_1}$$

$$u_1 = K_{1,real}([CO]_0 + [H_2O]_0) + ([CO_2]_0 + [H_2]_0)$$

$$v_1 = K_{1,real}([CO]_0[H_2O]_0) - ([CO_2]_0[H_2]_0)$$

$$K_{1,real} = \exp(\frac{8240}{T_1 + 459.67} - 4.33)$$

The volume of the low temperature catalyst is given by

$$V_2 = \frac{VF_2}{SV_2}$$

where

$$\frac{k_2}{SV_2} = \frac{K_{2,real}}{\sqrt{q_2}}\left\{\ln[\frac{2w_2x_2 - u_2 - \sqrt{q_2}}{2w_2x_2 - u_2 + \sqrt{q}_2} - \ln[\frac{-u_2 - \sqrt{q_2}}{-u_2 + \sqrt{q_2}}]\right\}$$

where $w_2 = K_{2,real} - 1$

$$\sqrt{q_2} = \sqrt{u_2{}^2 - 4w_2v_2}$$

$$u_2 = K_{2,real}([CO]_0 + [H_2O]_0 - 2x_1) + ([CO_2]_0 + [H_2]_0 + 2x_1)$$

$$v_2 = K_{2,real}[([CO]_0 - x_1)([H_2O]_0 - x_1)] - [([CO_2]_0 + x_1)([H_2]_0 + x_2)]$$

$$K_{2,real} = \exp(\frac{8240}{T_2 + 459.67} - 4.33)$$

For the iron-based catalyst, the reaction rate constant is given by,

$$\log(\frac{k_1}{A_p}) = 6.947 - \frac{3830}{0.85T_1 + 0.15T_0 + 459.67}$$

For the copper-based catalyst, the reaction rate constant is given by [6]

$$\log(\frac{k_2}{A_p}) = 6.91 - \frac{3062}{0.85 \cdot T_2 + 0.15 \cdot 450 + 459.67}$$

Here A_p is pressure-dependent activity factors, which can be given by

$$p \le 400 psig \ , A_p = 4 \cdot 10^{-8} p^3 + 10^{-5} p^2 + 0.0092 p + 0.9984$$

$$p \succ 400 psig \ , A_p = 4$$

Here the unit of pressure p is Psia.

Based on the volume of catalyst, the process facility costs of the high and low temperature shift reactors are regressed as a function of reactor volume.

$$C_{reactor} = 0.9927 \cdot N_T [17.6487(\frac{1.2V}{N_T})^{0.4883} P^{2.028}]$$

$C_{reactor}$—PFC cost of reactor (US$ in 2000)

V—volume of catalyst (m^3), 9~35 /train

N_T—number of trains

P—pressure (atm)

In this model, three heat exchangers are used. Heat exchanger 1 is gas-liquid type. It is used after the high temperature water gas shift reactor to cool down the syngas to 450F. At the same time, the saturation water at the pressure of the steam cycle is generated. its PFC cost was regressed by,

$$C_{h1} = 1.0064 \cdot N_T \cdot [13.7528 (dT)_1^{-0.6714} (\frac{Q_1}{N_T})^{0.6855}]$$

C_{h1}—PFC cost of heat exchanger 1(1000 US$ in 2000)

Q_1—heat load of exchangers (kW), 1300~21000 /train

dT_1—long mean temperature difference, 50~190 C

N_T—number of trains

P—pressure (atm) 18~157

The inlet hot fluid temperature is $T_{h,i} = T_1$

The outlet hot fluid temperature $T_{h,o}$ is 450 F.

The inlet cold fluid temperature is $T_{h,o}$ 57 F.

The outlet cold fluid temperature is $T_{c,o}(F) = T_{w,sat}$

Heat exchanger 2 is gas-gas type. It is used after the low temperature reactor to heat up and wet the fuel gas after a SELEXOL process. The cold fuel gas (57F) is heated up to 400F, and wetted by adding cold water (57F). Its PFC cost is given by

$$C_{h2} = 0.9927 \cdot N_T [24.4281 p_2^{0.2804} (dT)_2^{-0.1143} (\frac{Q_2}{N_T})^{0.3881}]$$

C_{h2}—direct cost (1000 US$ in 2000)

Q_2—heat load of exchangers (kW), 1200~96000 /train

dT_2—long mean temperature difference, 10~340 C

N_T—number of trains

P—pressure (atm) 19~68

The inlet hot fluid temperature is $T_{h,i} = T_2$

The outlet hot fluid temperature is $T_{h,o} = T_{h2,o}$

The inlet cold fluid temperature $T_{c,o}$ is T_{fuel} (the default value is 57F).

The outlet cold fluid temperature $T_{c,o}$ is 400F.

Heat exchanger 3 is a gas-liquid type. It is used after the low temperature reactor to cool down the syngas to 100F. The heat is recovered to heat the cold water for the steam recycle. The cold water (57F) is heated up to a certain degree to keep the log mean temperature difference at 40 F. Its PFC cost is given by

$$C_{h3} = 1.0064 \cdot N_T \cdot [13.7528(dT)_3^{-0.6714}(\frac{Q_3}{N_T})^{0.6855}]$$

C_{h3}—PFC cost of heat exchanger 1(1000 US$ in 2000)

Q_3—heat load of exchangers (kW), 1300~21000 /train

DT_3—long mean temperature difference, 50~190 C

N_T—number of trains

P—pressure (atm) 18~157

4.2 Selexol cost parameters

Capital cost elements	Nominal value
Total process facilities cost	Sum of the above value
Engineering and home office	10% PFC
General facilities	15% PFC
Project contingency	15% PFC
Process contingency	5% PFC
Total plant cost (TPC) = sum of above	
Interest during construction	Calculated
Royalty fees	0.5% PFC
Preproduction fees	1 moth fee of VOM&FOM
Inventory cost	0.5% TPC
Total capital requirement (TCR) = sum of above	
Fixed O&M cost (FOM)	
Total maintenance cost	2% TPC
Maintenance cost allocated to labor	40% of total maintenance cost

Administration & support labor cost	30% of total labor cost
Operation labor	1 jobs/shift
Variable O&M cost (VOM)	
High temperature catalyst	\$50/ft^3
Low temperature catalyst	\$250/ft^3

Reference

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Appendix B

Performance and cost model of Selexol process for CO_2 capture

1. Introduction to Selexol absorption process

Selexol is a commercially available physical solvent which is a mixture of dimethyl ether and polyethylene glycol [1]. It is widely used in physical absorption processes for acid gases treatment, such as H_2S removal and bulk CO_2 capture. A general scheme of Selexol process for CO_2 capture is given in Figure 1.

CO_2 from the cooled, shifted syngas is absorbed by the lean solvent at a high temperature in counter flow form. The pressure energy in the rich solvent is recovered with one or two hydro turbines. Most of the H_2 and CH_4 entrained and absorbed in the solvent is released in the slump tank and recycled to the absorber. Little CO_2 is released because of a large amount of excess glycol solvent introduced in the absorber. The majority of CO_2 absorbed by the solvent is recovered through flashing. The lean solvent is compressed and cooled down and fed into the absorber.

The heat demand for solvent regeneration in the Selexol process is zero because solvent recovery is possible through flashing. As a result the net power loss associated with the Selexol-based CO_2 capture is less than the other CO_2 recovery systems, such as Amine system [2-8].

2. Properties of Glycol solvent

The general properties of Glycol solvent is given in Table 1[9-10].

Table 1. Property of Glycol solvent

Solvent cost $/lb	1.32
Licensor	Norton
Viscosity @25C,cp	5.8
Specific gravity@25C,kg/m^3	1030
Mole weight	280
Vapor pressure @25C, mmHg	0.00073
Freezing point C	-28
Maximum operating Temp., C	175
Specific heat@25C Btu/lb F	0.49
CO_2 solubility SCF/US gal @25C	0.485

Number of commercial plants	32

The solubility of acid gases in Glycol depends on partial pressure and temperature. The solubility of CO_2 at 25C is 0.0375 SCF/gallon solvent. The relative solubilities of other gas are given in Table 2 [11].

Table 2. The relative solubility of gases in Selexol solvent.

Gas	CO_2	H_2	CH_4	CO	H_2S	COS	SO_2	NH_3	N_2	H_2O
Solubility (scf/gallon)	1	0.013	0.0667	0.028	8.93	2.33	93.3	4.87	0	733

The solubility of CO_2 as a function of temperature is regressed and given by

$$c = 0.0908 - 0.0008 \cdot T \quad (1)$$

The temperature range for the above equation is 30~77F.

The solubilities of other gases at different temperature are not available. Hence, here the relative solubilities of other gases at different temperature are assumed to be constants.

3. Performance model of Selexol process

The input and output parameters of this model are given in Table 3. For the performance simulation, the first step is to calculate the flow rate of the Glycol solvent. In order to do this calculation, the whole Selexol process can be simplified as Figure 3. Stream 1 is the syngas fed into the absorber at a given temperature. a percent of CO_2 is removed from the syngas and the final fuel gas temperature is 30F. Stream 4 is the lean solvent at temperature 30F. Due to heat transfer between the solvent and syngas and the absorption heat, the temperature of the rich solvent (stream 3) will be increased by ΔT. For the given CO_2 removal percentage a, the flow rate of glycol solvent, fuel gas and CO_2 product can be calculated as follows.

3.1 Flow rate calculation

3.1.1 Solvent flow rate

Assuming the flow rate of solvent is w lb-mol/hr, the temperature increase of solvent in the absorber is given by

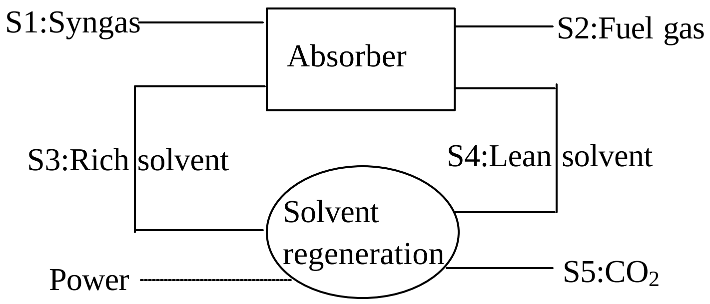
$$\Delta T = \Delta T_1 + \Delta T_2 \quad (2)$$

In the above equation, ΔT_1 is caused by the heat transfer, which can be estimated by

Table 3. Input and output parameters of Selexol model

Input parameter				Output parameter		
Syngas input	Flow rate (mole/s)	f_1		Fuel gas output	Flow rate (mole/s)	f_2
	Pressure	p_1			Pressure	p_2
	Temperature	T_1			Temperature	T_2
	Molar concentrations	$[CO]_1$			Molar concentrations	$[CO]_2$
		$[CO_2]_1$				$[CO_2]_2$
		$[H_2]_1$				$[H_2]_2$
		$[CH_4]_1$				$[CH_4]_2$
		$[H_2S]_1$				$[H_2S]_2$
		$[COS]_1$				$[COS]_2$
		$[NH_3]_1$				$[NH_3]_2$
		$[H_2O]_1$				$[H_2O]_2$
CO_2 removal percentage				CO_2 flow	Flow rate (mole/s)	f_5
					Pressure	P_5
				Refrig. power	Power recovery	Comp. power

Figure 2. Selexol process



$$\Delta T_1 = \frac{Q_1}{w \cdot MW_s \cdot C_{p,s}} \quad (3)$$

where MW_s is the molar weight of Selexol (0.28 lb/lb-mol);

$C_{p,s}$ is the specific heat of Selexol (0.49 Btu/lb F)

Q_1 is the heat released by the syngas, which can be estimated by,

$$Q_1 = 25 f_1\{2.02\cdot[H_2]_1\cdot C_{p,H_2} + 16\cdot[CH_4]_1\cdot C_{p,CH_4} + 28\cdot[CO]_1\cdot C_{p,CO} + 44\cdot[CO_2]_1\cdot(1-a)\cdot C_{p,CO_2}\} + 44\cdot(25-\Delta T)\cdot f_1\cdot a\cdot[CO_2]_1\cdot C_{p,CO_2} \quad (4)$$

The specific heat of the gases is given in Table 4.

Table 4. Specific heat of gases

Gas	CO	CO_2	H_2	CH_4	Ar	N_2	H_2S	NH_3
Specific heat (Btu/lb F)	0.248	0.199	3.425	0.593	0.125	0.249	0.245	0.52

In Eq. 2, ΔT_2 is caused by the solution heat. Here only the solution heat of CO_2 is calculated, and the solution heat of other gases is negligible.

$$\Delta T_2 = \frac{44 f_1\cdot[CO_2]_1\cdot a\cdot y}{w\cdot MW_s\cdot C_{p,s}} \quad (5)$$

where y is the solution heat of CO_2. The solution heat of several gases is given in Table 5 [10].

Table 5. The solution heat of gases

Gas	CO_2	H_2S	CH_3
Heat of solution (Btu/lb solute)	160	190	75

In the flash tanks, the residual time is long enough to assume that equilibrium can be achieved in these tanks. In the last flash tank, the solvent temperature is about (30+ΔT_1), hence the flow rate of residual CO_2 in the lean solvent (S4 in figure 3) can be given by

$$V_{CO_2,res}(SCF/hr) = 32.574 w\cdot p_{CO_2} c_{CO_2,4} \quad (6)$$

$$m_{CO_2,res}(lb\cdot mol/hr) = \frac{V_{CO_2,res}}{377.052} \quad (7)$$

where 32.574 is the specific volume of Selexol (gallon/lb-mol);

377.052 is the specific volume of CO_2 (SFC/lb-mol)

w is the flow rate of Selexol (lb-mol/hr);

p_{CO_2} is the partial pressure of CO_2 (psia);

$c_{CO_2,4}$ is the solubility of CO_2 in Selexol at temperature of 30+ ΔT_1 (F).

In the absorber, the amount of CO_2 that need be captured by the solvent is

$$V_{CO_2,abs}(SCF/hr) = 377.052 f_1 \cdot [CO_2]_1 \cdot a \qquad (8)$$

In the absorber, the equilibrium cannot be achieved due to limited residual time. The flow rate of solvent used in the absorber is larger than that of the solvent required to capture a percentage of CO_2 at equilibrium. The ratio of the flow rate of the solvent was regressed based on some references [11-13].

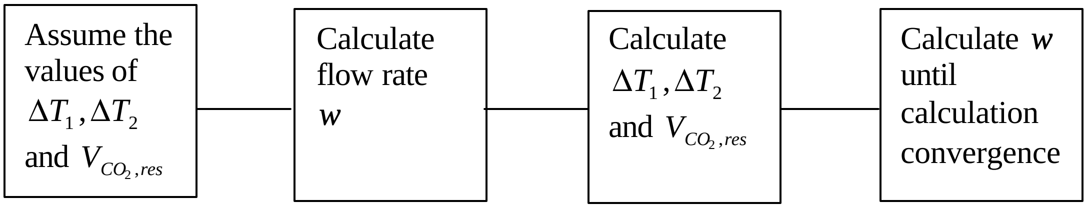
$$g = 1.55 - 0.0002 p_1 \qquad (9)$$

Then the flow rate of Selexol needed to capture a percentage of CO_2 is given by

$$w(lb \cdot mol/hr) = \frac{g\,(V_{CO_2,res} + V_{CO_2,abs})}{32.574 p_1 \cdot [CO_2]_1 \cdot c_{CO_2,1}} \qquad (10)$$

where $c_{CO_2,1}$ is the solubility of CO_2 in Selexol at temperature of 30+ ΔT F.

Based on the above discussion, the calculation process for the flow rate of Selexol is represented by the following figure,



3.1.2 Composition of and flow rate of fuel gas

After CO_2 capture, syngas is converted into fuel gas, the main component of which is hydrogen. The composition and flow rate of fuel gas can be calculated as follows.

With known Selexol flow rate and solubility of gases, the volume and mass amount of species i which is captured by the solvent is

$$V_i(SCF/hr) = 32.574 w \cdot p_i c_i \qquad (11)$$

$$m_i(lb \cdot mol/hr) = \frac{V_i}{v_i} \tag{12}$$

where 32.574 is the specific volume of Selexol (gallon/lb-mol);

v_i is the specific volume of CO_2 (SFC/lb-mol)

w is the flow rate of Selexol (lb-mol/hr);

p_i is the partial pressure of species i, here is 4psia;

c_i is the solubility of species i in Selexol at temperature of 30+ ΔT F.

In the slump tank, almost all of the H_2, CO and CH_4 in the Selexol are released and recycled to the absorber again. Because of a large amount of extra Selexol is used in the absorber, only a small amount of CO_2 is released in the slump tank. Based on the data in references [8-9], 1% of CO_2 in the solvent is assumed to be released and recycled to the absorber.

3.1.3 Composition and flow rate of CO_2 rich flow

At the last stage, the flash pressure is given. At this pressure, the residual gases in the lean solvent can be calculated based on their solubility. Based on mass conservation, the composition and flow rate of CO_2 rich flow can be calculated. To simplify, all the gases except CO_2 are assumed to be released from the solvent at the flash tanks.

3.2 Power consumption

There is no heat duty in the Selexol process because the solvent is regenerated through pressure flashing, but power input is required to compress the recycling gas from the slump tank, the lean solvent from the flash tank 3, and CO_2 rich product. At the same time, some electricity can be generated through the power recovery hydro turbine. The total power consumption is the difference between the power input and the recovered power.

3.2.1 Power recovery

In this performance model, the pressure of the high-pressure rich solvent from the absorber is reduced and the energy is recovered through one or two hydro turbines. Here if the system pressure is larger than 240psia, two power recovery turbines will be used. Otherwise, only one power recovery turbine will be used. The outlet pressure of the first power recovery turbine is selected to make most of the less soluble gases, such as H_2, CO and CH_4 released while avoiding release of CO_2. Generally, this outlet pressure can be determined based on the system pressure as following:

$$p_{o,1} = 0.0402 p_1^{1.415} \quad (150 \leq p_1 \leq 1000) \tag{13}$$

If the system pressure is larger than 240 psia, then the outlet pressure of the second turbine is given by

$$p_{o,2} = 35.619 \ln(p_1) - 169.88 \quad (150 \leq p_1 \leq 1000) \tag{14}$$

The power recovered from the liquid solvent is calculated from the following expression

$$hydraulic \quad hp = H_s \cdot \frac{G}{1714} \cdot h \tag{15}$$

where H_s is the total dynamic head (lb/in^2);

G is the flow rate of liquid (gal/min);

h is the efficiency of the turbine.

The temperature change of the solvent in the turbine can be calculated based on change in enthalpy, which equals flow work, $\int vdp$. For the default efficiency of turbines, 78%, the temperature can be given by

$$dT = 0.0047 \cdot \Delta p - 0.0715 \tag{16}$$

where dT (F)is the temperature decreased in the power recovery turbine;

Δp (psia)is the pressure decreased in the power recovery turbine.

3.3.2 CO_2 compression

There are three flashing pressure levels. If the system pressure is larger than 240psia, the first flashing pressure equals the outlet pressure of the second turbine. If the system pressure is less than 240psia, the first flashing pressure is set to be 25psia. The second flashing pressure is set to be 14.7psia, and the last flashing pressure is set to be 4 psia.

In flashing tank 1, the less soluble gases CO, H_2 and CH_4 are assumed to be totally released from the solvent. The amount of CO_2 released in this tank can be calculated based on Eq 1. In flashing tank 2 and 3, the amount of CO_2 released can also be calculated using Eq. 1. CO_2 from the flash tank 2 and tank 3 is compressed to the flashing pressure of tank 1. The change in temperature of the solvent is due to the release of CO_2. The CO_2 will finally be compressed to high pressure (>1000psia) for storage using a multi-stage, inter-stage cooling compressor. The power required by carbon dioxide gas compressors is estimated by using the expression [12].

$$hp = \frac{0.00436}{\eta} \cdot Q_1 \cdot p_{in} \cdot \left(\frac{k}{k-1}\right) \cdot \left[\left(\frac{p_o}{p_{in}}\right)^{(k-1)/k} - 1\right] \tag{17}$$

where Q_1 is the inlet rate of gases (ft^3/min);

p_i is the inlet pressure (psia);

p_o is the outlet pressure (psia);

$$k = C_p / C_v = 1.395$$

η is the overall efficiency of compressor (default value is 82%).

3.3.3 Solvent compression work

The lean solvent is pumped back to the absorber operating pressure by using a circulation pump. The power required by the circulation pump is estimated by[12]

$$pump \quad hp = H_s \frac{G}{1714\eta} \tag{18}$$

where H_s is the total dynamic head (psia);

G is the flow rate of liquid (gal/min);

η is the efficiency of the turbine.

The increase in temperature of the solvent due to the heating of pumping can be calculated by

$$dT = 0.0082 \cdot \Delta p - 0.3093 \qquad (19)$$

where dT (F)is the temperature increase due to pumping;

Δp (psia)is the pressure increase in the pump.

3.3.4 Recycle gas compression work

The gases from the slump tank are recycled to the absorber. A compressor is used to compress the gases to the operating pressure of the absorber. The power of the compressor is estimated using Eq. 19.

3.3.5 Solvent refrigeration

The temperature of the solvent increases due to heat transfer in the absorber, the heat of absorption and pumping. The solvent has to be cooled down to the absorber operating temperature (30F) by using refrigeration. The refrigeration power is estimated by

$$refrigeration \quad power(kW) = \frac{refrigeration \quad load(Btu/hr)}{1000(9 + {}^{T_{evap}}\!/_{10})} \qquad (20)$$

where the refrigeration load equals the enthalpy change of the solvent.

T_{evap} is the evaporation temperature of refrigerant.

3.4 Makeup of Selexol solvent

The vapor pressure of the Selexol solvent is 1.35×10^{-5} psia at 77F, which is very low. The real vapor pressure is even lower because the operating temperature is usually lower than 77F. Hence, the loss of solvent due to evaporation is negligible.

4. Cost model of Selexol process

The cost outputs of this model include total plant cost, total plant investment, total capital requirement, operation and maintenance cost.

4.1. Total Plant Cost (TPC)

The total plant cost is the sum of the process facilities capital (PFC), general facilities capital (GFC), engineering and home office fee, and contingencies including project contingency and process contingency.

4.1.1 The PFC for this Selexol absorption system includes:

CO_2 absorption column

$$C = 0.99989 \ N_T \cdot [-1375.356 + 16.536 \ P_{in} + 0.127628 \ (0.5 f_{SEL} + 0.5 f_{gas}) \qquad (21)$$

C—PFC cost (1000 US$ in 2000)

f_{SEL} --flow rate of Selexol(lb-mol/h)

f_{gas} --flow rate of gas captured in Selexol (lb-mol/h)

N_T—number of trains

P_{in}—inlet pressure (atm)

Power recovery turbine

$$C = 219.086 + 0.080912 \cdot hp + 0.020086 p_{out}^2 \qquad (24)$$

C—PFC cost (1000 US$ in 2000)

hp—horse power of turbine

P_o—outlet pressure of turbines (atm)

Slump tank

$$C = 2.0049 \cdot N_T \cdot (\frac{F}{N_T})^{0.7446} \qquad (25)$$

C—PFC cost (1000 US$ in 2000)

F--flow rate of solvent (kg/s), 400~800/train

N_T—number of trains

Pressure arrange: 3~50 atm

Recycle compressor

$$C = 4.45519 hp^{0.778385} \quad (26)$$

C—PFC cost (1000 US$ in 2000)

hp-- horse power of turbine

Selexol pump

$$C = 1.22864 hp^{0.7164} \quad (27)$$

C—PFC cost (1000 US$ in 2000)

hp-horse power of compressor

CO_2 compressor

$$C = 7.0321 hp^{0.6769} \quad (28)$$

C—PFC cost (1000 US$ in 2000)

hp-horse power of compressor

CO_2 final product compressor

$$C = 13.0969 hp^{0.64} \quad (29)$$

C—PFC cost (1000 US$ in 2000)

hp-horse power of compressor

Refrigeration

$$C = 1.0019 \cdot N_T \cdot [16.4796 \cdot (\frac{F}{N_T})^{0.3618} (\Delta T)^{0.4064}] \quad (30)$$

C—PFC cost (1000 US$ in 2000)

F--flow rate of solvent(lb-mol/h), 70000~23000 /train

N_T—number of trains

ΔT --temperature difference between the inlet and outlet solvent (C), 1~5

Flash tank

$$C = 0.9832 \cdot N_T (\frac{F}{N_T})^{0.8005} \tag{30}$$

C—PFC cost (1000 US$ in 2000)

F--flow rate of glycol(kg/s), 400~800 /train

N_T—number of trains

Heater exchanger

The FPC of gas-gas heater exchanger is given by

$$C \ = 0.9927 \cdot N_T [24.4281 p^{0.2804} (dT)^{-0.1143} (\frac{Q}{N_T})^{0.3881}] \tag{31}$$

C—direct cost (1000 US$ in 2000)

Q—heat load of exchangers (kW), 1200~96000 /train

dT—long mean temperature difference (based on C), 10~340 C

N_T—number of trains

P—pressure (atm) 19~68

The inlet hot fluid temperature is $T_{h,i} = 100F$

The outlet hot fluid temperature is $T_{h,o} = 55F$

The inlet cold fluid temperature $T_{c,o}$ = 30F.

The outlet cold fluid temperature $T_{c,o}$ is calculated based on energy conservation.

4.2 Selexol cost parameters

Capital cost elements	Nominal value
Total process facilities cost	Sum of the above value
Engineering and home office	10% PFC
General facilities	15% PFC
Project contingency	15% PFC

Process contingency	10% PFC
Total plant cost (TPC) = sum of above	
Interest during construction	Calculated
Royalty fees	0.5% PFC
Preproduction fees	1 moth fee of VOM&FOM
Inventory cost	0.5% TPC
Total capital requirement (TCR) = sum of above	
Fixed O&M cost (FOM)	
Total maintenance cost	2% TPC
Maintenance cost allocated to labor	40% of total maintenance cost
Administration & support labor cost	30% of total labor cost
Operation labor	2 jobs/shift
Variable O&M cost (VOM)	
Selexol solvent	$ 1.96/lb

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Appendix C

Input parameters and output results of the reference IGCC plant

Reference plant: coal-fueled Texaco entrained flow IGCC power plant with total quench high temperature gas cooling--system summary

Gasifier conditions		
Dry coal flow rate:	355940.47	lb/hr
Oxygen flow rate:	337249.91	lb/hr
Water flow rate:	184337.12	lb/hr
Gasifier pressure:	615	Psia
Gasifier temperature:	2400	F
MS7000 gas turbine conditions		
Fuel flow rate:	1106834.4	lb/hr
Air flow rate:	6043824.8	lb/hr
Fuel HHV:	3152.6	Btu/lb
Firing temperature:	2335	F
Combustion exit temperature:	2410.4	F
Turbine exhaust temperature:	1123.7	F
Generator efficiency:	0.985	
Steam turbine conditions		
Superheated steam flow rate:	775008.54	lb/hr
Superheated steam temperature:	992.9	F
Reheat steam temperature:	993.1	F
Expanded steam quality:	0.935	
Generator efficiency:	0.985	
Power productity summary		
Gas turbine:	388.2	MW
Steam turbine:	185.4	MW
Performance summary		
Oxygen blown Texaco-based IGCC system with cold gas cleanup		
Cost model input performance parameters		
Mass flow of coal to gasifier	355940.5	lb/hr
Ambient temperature	59.0	F
Oxidant feedrate to gasifier	10539.1	lbmole/hr
Oxygen flow to gasifier	10012.1	lbmole/hr
Molar flow of syngas to LTGC	33921.1	lbmole/hr
Syngas temperature in LTGC	101.0	F
Syngas pressure in LTGC	537.0	psia
H2S entering Selexol unit	0.0	lbmole/hr
Syngas entering Selexol unit	33921.1	lbmole/hr

Mass flow of raw water	483528.3	lb/hr
Mass flow of polished water	1273587.0	lb/hr
Mass flow of scurrber blowdown	834381.8	lb/hr
Gas turbine power	711.5	MW
Gas turbine compressor	323.3	MW
Pressure of HP steam (HRSG)	1465.0	psia
Mass flow of HP steam (HRSG)	775008.5	lb/hr
Steam trubine power	188.2	MW
Heating value of coal (HHV)	13126.0	Btu/lb
Waste water flow rate	834381.8	lb/hr
Steam cycle pump	2.8	MW
Blowdown	40786.7	lb/hr

Cost summary

A. Cost model parameters

Plant capacity factor:	0.75	Cost year	2000yr
General facilities factor:	0.15	Levelization cost factor:	1
Indirect construction:	0.2	Escalations	0
Sales tax:	0.05	Interest:	0.1
Engr&Home office Fee:	0.1	Years of construction:	4
Project contingency:	0.125	Average labor rate:	19.7
Number of shifts:	4.25	Book life (years)	30

B. Process contingency and maintance cost factors

Plant section	Process contingency	Maintance cost factor
Coal handling:	0.05	0.03
Oxidant feed	0.05	0.02
Gasification	0.15	0.045
LTGC	0	0.03
Selexol	0.1	0.02
Claus plant	0.05	0.02
Beavon-Stretford	0.1	0.02
Boiler feedwater treatment	0	0.015
Process condensate treatment	0.3	0.02
Gas turbine	0.125	0.015
HRSG	0.025	0.015
Steam turbine	0.025	0.015
General facilities	0.05	0.015

C. Direct capital and process contingency costs ($1000)

Plant section	Number of operating	Direct capital cost	Process contingency

Coal handling:		1	23486.2	1174.3
Oxidant feed		1	73731.4	3686.6
Gasification		3	33266.7	4990.0
LTGC		1	19143.6	957.2
Selexol		1	9607.5	960.7
Claus plant		2	4783.2	239.2
Beavon-Stretford		1	5030.2	503.0
Boiler feedwater treatment		1	4046.3	202.3
Process condensate treatment		1	3248.6	974.6
Gas turbine		2	70969.0	8871.1
HRSG		2	19030.1	475.8
Steam turbine		1	31276.4	781.9
General facilities	N/A		44642.9	2232.1
Total direct cost			342262.3	26048.8

D. Total capital requirement ($1000)

Indirect construction cost	68452.5
Sales tax	17113.1
Engineering and home office fees	34226.2
Environmental permitting	1000.0
	120791.8
Total process contingencies	26048.8
Project contingency	64174.2
TPC	553277.1
AFDC	71321.2
TPI	624598.3
Preproduction (startup) costs	15615.0
Inventory capital	624.6
Initial catalysts and chemicals	5621.4
Land	1731.2
TCR	648190.5

E. Fixed operating cost ($/yr)

Operating labor	4532908.0
Maintenance costs	13236790.3
Administration and supervision	2916962.5

F. Variable operating costs

	unit cost		Material requirement		Annual cost
Sulfuric acid	119.52	$/ton	1143.2	ton/yr	136630.5
NaOH	239.04	$/ton	236.3		56489.8
Na2 HPO4	0.76	$/lb	1180.8		897.4
Hydrazine	3.48	$/lb	5681.5		19771.5
Morpholine	1.41	$/lb	5292.6		7462.5

Lime	86.92	$/ton	392.7		34131.4
Soda ash	173.85	$/ton	433.9		75433.2
Corrosion Inh	2.06	$/lb	78285.7		161268.6
Surfactant	1.36	$/lb	78285.7		106468.6
Chlorine	271.64	$/ton	12.2		3305.1
Biocide	3.91	$/lb	13497.6		52775.5
Selexol Solv.	1.96	$/lb	34741.8		68094.0
Claus catalyst	478.08	$/ton	7.8		3733.2
B/S catalyst	184.71	$/ft^3	38.4		7088.7
B/S chemicals					82851.7
Fuel oil	45.64	$/bbl	27229.4		1242750.7
Plant air ads.	3.04	$/lb	2042.2		6208.3
Water	0.79	$/Kgal	330311.9		260946.4
Waste water	912.7	$/gpm	835088.9		1635123.0
LPG-flare	12.71	$/bbl	2382.6		30282.4
Total consumables ($/yr)					3991712.5
Fuel, ash disposal, and byproduct credit ($/yr)					
Coal	1.26	$/MMBtu	355940.5	lb/hr	38676371.3
Ash disposal	10.87	$/ton	434.9	ton/day	1190447.9
Byprod. Credit	75	$/ton	6.6	ton/hr	3251195.5
Total variable operating cost ($/yr)					43858531.7
G. Cost of electricity					
Power summary (Mwe)					
Coal handling	4.03				
Oxidant feed	52.00				
Gasification	0.64				
Low T Cool	1.49				
Selexol for H2S	0.70				
Claus	0.26				
B/S	0.82				
Proc. Cond	0.14				
Steam cycle	2.80				
General Fac	6.29				
Total auxiliary loads	69.16				
Net electricity	504.5				
Capital cost	1284.9				
COE	39.70				
Heat rate,Btu/kWh	9261.60				
Efficiency	0.368				

Input parameters and output results of the IGCC plant with CO_2 capture

IGCC plant with CO_2 capture: coal-fueled Texaco entrained flow IGCC power plant with total quench high temperature gas cooling: system summary

Gasifier conditions

Dry coal flow rate:	355940.5	lb/hr
Oxygen flow rate:	337249.9	lb/hr
Water flow rate:	184337.1	lb/hr
Gasifier pressure:	615.0	Psia
Gasifier temperature:	2400.0	F

MS7000 gas turbine conditions

Fuel flow rate:	225143.5	lb/hr
Air flow rate:	5050000.0	lb/hr
Fuel HHV:	14101.7	Btu/lb
Firing temperature:	2335.0	F
Combustion exit temperature:	2410.0	F
Turbine exhaust temperature:	1123.7	F
Generator efficiency:	0.985	

Steam turbine conditions

Superheated steam flow rate:	788078.9	lb/hr
Superheated steam temperature:	992.9	F
Reheat steam temperature:	993.1	F
Expanded steam quality:	0.935	
Generator efficiency:	0.985	

Power productity summary

Gas turbine:	370.9	MW
Steam turbine:	190.8	MW

Performance summary

Oxygen blown Texaco-based IGCC system with cold gas cleanup

Cost model input performance parameters

Mass flow of coal to gasifier	355940.5	lb/hr
Ambient temperature	59.0	F
Oxidant feedrate to gasifier	10539.1	lbmole/hr
Oxygen flow to gasifier	10012.1	lbmole/hr
Molar flow of syngas to LTGC	33921.1	lbmole/hr
Syngas temperature in LTGC	101.0	F
Syngas pressure in LTGC	537.0	psia
Syngas entering Selexol unit	33921.1	lbmole/hr

Mass flow of raw water	483528.3	lb/hr
Mass flow of polished water	1273587.0	lb/hr
Mass flow of scurrber blowdown	834381.8	lb/hr
Gas turbine power	9.8	MW
Gas turbine compressor	269.0	MW
Pressure of HP steam (HRSG)	1465.0	psia
Mass flow of HP steam (HRSG)	788090.8	lb/hr
Steam trubine power	193.8	MW
Heating value of coal (HHV)	13126.0	Btu/lb
Waste water flow rate	834381.8	lb/hr
Steam cycle pump	3.0	MW
Blowdown	40786.7	lb/hr

Cost summary

Oxygen blown Texaco-based IGCC system with cold gas cleanup

A. Cost model parameters

Plant capacity factor:	0.75	Cost year	2000yr
General facilities factor:	0.15	Levelization cost factor	1
Indirect construction:	0.2	Escalations	0
Sales tax:	0.05	Interest:	0.1
Engr&Home office Fee:	0.1	Years of construction:	4
Project contingency:	0.15	Average labor rate:	19.7
Number of shifts:	4.25	Book life (years)	30

B. Process contingency and maintance cost factors

Plant section	Process contingency	Maintance cost factor
Coal handling:	0.05	0.03
Oxidant feed	0.05	0.02
Gasification	0.15	0.045
LTGC	0.05	0.03
WGS	0.05	0.02
Selexol for H_2S capture	0.1	0.02
Claus plant	0.05	0.02
Beavon-Stretford	0.1	0.02
Selexol for CO_2 capture	0.1	0.05
Boiler feedwater treatment	0.05	0.015
Process condensate treatment	0.3	0.02
Gas turbine	0.125	0.015
HRSG	0.025	0.015
Steam turbine	0.025	0.015

General facilities	0.05	0.015

C. Direct capital and process contingency costs ($1000)

Plant section	Number of operating	Direct capital cost	Process contingency
Coal handling:	1	23486.2	1174.3
Oxidant feed	1	73731.4	3686.6
Gasification	3	33266.7	4990.0
LTGC	1	19143.6	957.2
WGS	3	29807.3	1490.4
Selexol	1	9607.5	960.7
Claus plant	2	4783.2	239.2
Beavon-Stretford	1	5030.2	503.0
Selexol for CO_2 capture	3	42900.4	4290.0
Boiler feedwater treatment	1	4046.3	202.3
Process condensate treatment	1	3248.6	974.6
Gas turbine	2	70969.0	8871.1
HRSG	2	19129.2	478.2
Steam turbine	1	31817.4	795.4
General facilities	N/A	44738.9	2236.9
Total direct cost		415705.9	31850.0

D. Total capital requirement ($1000)

Indirect construction cost	83141.2
Sales tax	20785.3
Engineering and home office fees	41570.6
Environmental permitting	1000.0
	146497.1
Total process contingencies	31850.0
Project contingency	77944.9
TPC	671997.9
AFDC	86625.2
TPI	758623.1
Preproduction (startup) costs	18965.6
Inventory capital	758.6
Initial catalysts and chemicals	6827.6
Land	1790.0
TCR	786964.9
Fixed operating cost ($/year)	
Operating labor	5541903.1
Maintenance costs	18259237.1
Administration and supervision	3566258.9

F. Variable operating costs ($/year)

Description	unit cost		Material requirement		
Sulfuric acid	119.52	$/ton	1143.2	ton/yr	136630.5
NaOH	239.04	$/ton	236.3		56489.8
Na2 HPO$_4$	0.76	$/lb	1180.8		897.4
Hydrazine	3.48	$/lb	5681.5		19771.5
Morpholine	1.41	$/lb	5292.6		7462.5
Lime	86.92	$/ton	392.7		34131.4
Soda ash	173.85	$/ton	433.9		75433.2
Corrosion Inh	2.06	$/lb	78285.7		161268.6
Surfactant	1.36	$/lb	78285.7		106468.6
Chlorine	271.64	$/ton	12.2		3305.1
Biocide	3.91	$/lb	13497.6		52775.5
HT catalyst	50	$/ft^3			8212.9
LT catalyst	250	$/ft^3			6679.0
Selexol Solv.	1.96	$/lb	327998.6		642877.3
Claus catalyst	478.08	$/ton	7.8		3733.2
B/S catalyst	184.71	$/ft^3	38.4		7088.7
B/S chemicals					82851.7
Fuel oil	45.64	$/bbl	27229.4		1242750.7
Plant air ads.	3.04	$/lb	2042.2		6208.3
Water	0.79	$/Kgal	330311.9		260946.4
Waste water	912.7	$/gpm ww	835088.9		1635123.0
LPG-flare	12.71	$/bbl	2382.6		30282.4
Total consumables ($/yr)					4581387.7
Fuel, ash disposal, and byproduct credit ($/yr)					
Coal	1.26	$/MMBtu	355940.5	lb/hr	38676368.5
Ash disposal	10	$/ton	434.9	ton/day	1190447.9
Byprod. Credit	75	$/ton	6.6	ton/hr	3251195.5
Total variable operating cost ($/yr)					44123084.6

G. Cost of electricity

Power consuming (MW)	
Coal handling	4.03
Oxidant feed	52.00
Gasification	0.64
Low T Cool	1.49
Selexol for H_2S	0.70
Selexol for CO_2 capture	40.26
Claus	0.26
B/S	0.82
Proc. Cond	0.82
Steam cycle	3.00
General Fac	10.38
Total auxiliary loads	114.40

Net electricity	447.5
Capital cost	1758.6
CO2 storage, \$/ton CO_2	10
COE	60.33
Heat rate,Btu/kWh	10440.4
Efficiency	0.327

Appendix D

Methodology for encoding uncertainties as probability distributions

There are three general areas of uncertainty that have been explicitly reflected in this study. These are uncertainties in: (1) process performance parameters, (2) process area capital cost, and (3) process operating costs. Generally, developing the estimation of uncertainties in specific process parameters involves several steps. These include:

1. Review the technical basis for uncertainty in the process
2. Identify specific parameters that should be treated as uncertain
3. Identify the source of information regarding uncertainty for each parameter
4. Depending on the availability of information, develop estimates of uncertainty based on:

--Published judgments in the literature
--Published information that can be used to infer a judgment about uncertainty
--Statistical analysis of data
--Elicitation of judgments from technical expert

Reviewing the technical basis for uncertainty and identifying specific parameters that should be treated as uncertain had been completed with the development of the technical and economic models. Some of the probability distributions of parameters directly came from published judgments in the literature. For example, the distribution of CO_2 product pressure came from reference [1]. While most of the probability distributions were still encoded through statistical analysis of data from review of published information. Just as Professor Allen Robinson's comment, "sometimes taking histogram of literature values may provide a misleading estimate of uncertainty, because some published literature values may have little bearing on how system actual performances once it has been deployed." With this in mind, a much more attention was paid to collect data from project reports and papers published by industrial companies with real-world experiences. After data collection, the encoding process is as in the following.

Visualizing data

As the first step, the data set for each parameter was visualized through plotting the data in figures. The purposes of visualizing data sets include (1) evaluating the central tendency and dispersion of the data; (2) visually inspecting the shape of empirical data distribution as a potential aid in selecting parametric probability distribution models to fit to the data; (3) identifying possible anomalies in the data set (such as outliers); and (4) identifying possible dependencies between variables [2]. Specific techniques for evaluating and visualizing data include calculating summary statistics, developing empirical cumulative distribution functions using the general Blom's expression in Eq.1 [3], representing data using histograms, and generating scatter plots to evaluate dependencies between parameters.

$$F_X(x_i) = \Pr(X < x_i) = \frac{i-a}{n-2a+1} \qquad \text{for } i=1, 2,\ldots,n \text{ and } x_1<x_2<\ldots<x_n \qquad (1)$$

Selecting, fitting, and evaluating parametric probability distributions

In choosing a distribution function to represent uncertainty, a prior knowledge of the mechanism that impact a quantity play an important role. For example, one factor to consider may be whether values must be nonnegative.

In this study, most of the probability distributions were represents by uniform distribution or triangular distribution. Uniform probability is useful when it is possible to specify a finite rang of possible values, but is unable to decide which values in the range are more likely to occur than others. Triangle is similar to uniform except a mode is also specified. It is useful when we can specify both a finite range of possible values and a most likely (mode) value. For instance, for some input parameters, values toward the middle of the range of possible values are considered more likely to occur than values near either extreme. When this is the case, the triangular distribution provides a convenient means of representing uncertainty [4]. It is excellent for screening studies and easy to obtain judgments for. In addition to being simple, the shape of the uniform and triangular distributions can be a convenient way to send a signal that the details about uncertainty in the variable are not well known. This may help to prevent over-interpretation of results or a false sense of confidence in subtle details of results [4].

Once a particular distribution has been selected, a key step is to estimate the parameters of the distribution. The most widely used techniques for estimating the parameters are the method of maximum likelihood estimation (MLE), the method of least squares, and the method of matching moments [4]. MLE was used in this study when necessary.

The fitted parametric distributions may be evaluated for goodness of fit using probability plots and test statistics. In this study, the empirical distribution of the actual data set was compared visually with the cumulative probability functions of the fitted distributions to aid in evaluating the probability distribution model that described the observed data.

It may not always be possible to develop estimate of uncertainty based on classical statistical analysis. For example, I have only three data points about the temperature effect on the solubility of CO_2 in Selexol. With only three data points, there are a large number of parametric distribution families that would not be rejected by statistical tests. A uniform distribution was selected to represent the data. Therefore, the selection of a parametric distribution to represent the three data points is based upon judgment, rather than statistical analysis.

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