

# Synthetic fuel production by indirect coal liquefaction

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*This paper reports detailed process designs and cost assessments for production of clean liquid fuels (methanol and dimethyl ether) by indirect coal liquefaction (ICL). Gasification of coal produces a synthesis gas that can be converted to liquid fuel by synthesis over appropriate catalysts. Recycling of unconverted synthesis gas back to the synthesis reactor enables a larger fraction of the coal energy to be converted to liquid fuel. Passing synthesis gas once over the synthesis catalyst, with unconverted synthesis gas used to generate electricity in a gas turbine combined cycle, leads to less liquid fuel production, but provides for a significant second revenue stream from sale of electricity. Recently-developed liquid-phase synthesis reactors are especially attractive for “once-through” processing. Both “recycle” and “once-through” plant configurations are evaluated in this paper. Because synthesis catalysts are poisoned by sulfur, essentially all sulfur must be removed upstream. Upstream removal of CO<sub>2</sub> from the synthesis gas is also desirable to maximize synthesis productivity, and it provides an opportunity for partial decarbonization of the process, whereby the removed CO<sub>2</sub> can be captured for underground storage. The analysis here suggests that co-capture and co-storage of CO<sub>2</sub> and H<sub>2</sub>S (if this is proven technically feasible) could have important favorable impacts in some cases on liquid fuel production costs. Furthermore, the life-cycle CO<sub>2</sub> emissions from production and use of fuels made by ICL would be lower than with production and use of petroleum-derived transportation fuels. If CO<sub>2</sub> is not captured at ICL facilities, lifecycle CO<sub>2</sub> emissions to the atmosphere would be considerably higher than lifecycle emissions with petroleum-derived fuels.*

## 1. Introduction

For China, with abundant domestic coal resources but limited oil and gas resources, the conversion of coal into liquid fuels offers an alternative to importing petroleum or gas-based transportation fuels. Two routes to liquid fuels from coal include direct coal liquefaction (DCL) and indirect coal liquefaction (ICL). DCL, the production of a synthetic crude oil product by direct contact of coal with an appropriate catalyst in the presence of added hydrogen at elevated temperature, is discussed in a companion paper [Williams and Larson, 2003]. ICL is the production of fuels with an intermediate step of synthesis gas production by coal gasification. The principal constituents of “syngas” are carbon monoxide and hydrogen, which can be processed chemically into a variety of different fuels.

Fuels that can be made by ICL include methanol (CH<sub>3</sub>OH), dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub>), Fischer-Tropsch diesel- or gasoline-like fuels, and hydrogen (H<sub>2</sub>). The availability of CO and H<sub>2</sub> as molecular building-blocks at an ICL facility also provides opportunities for production of chemicals. Commercial application of ICL for fuel

production today exists in South Africa (for Fischer-Tropsch fuels). Also, the US Department of Energy announced its financial backing for a \$ 612 million project early this year to demonstrate advanced Fischer-Tropsch fuel production by ICL at a site in Pennsylvania<sup>[1]</sup>. In China, the production of methanol (primarily for use as chemical feedstock) by ICL processes is commercially established<sup>[2]</sup>. China has an estimated 10 to 15 modern coal gasification facilities in operation to make hydrogen for ammonia production. Also, there is considerable interest in China (especially Shanxi Province) in the use of methanol as a vehicle fuel [Niu, 2003]. There is also interest in pursuing ICL to produce dimethyl ether (DME) from coal: in 2002, China’s State Development Planning Commission approved plans for the first large-scale coal-to-DME project, to be located in Ningxia Province.

Dimethyl ether is a less familiar fuel option than methanol. It is used today exclusively as a chemical feedstock and aerosol propellant (e.g., in hair-sprays). DME is a potential premium fuel for compression ignition (diesel) engines because of its high cetane rating and because it burns without sooting since it contains no carbon-carbon

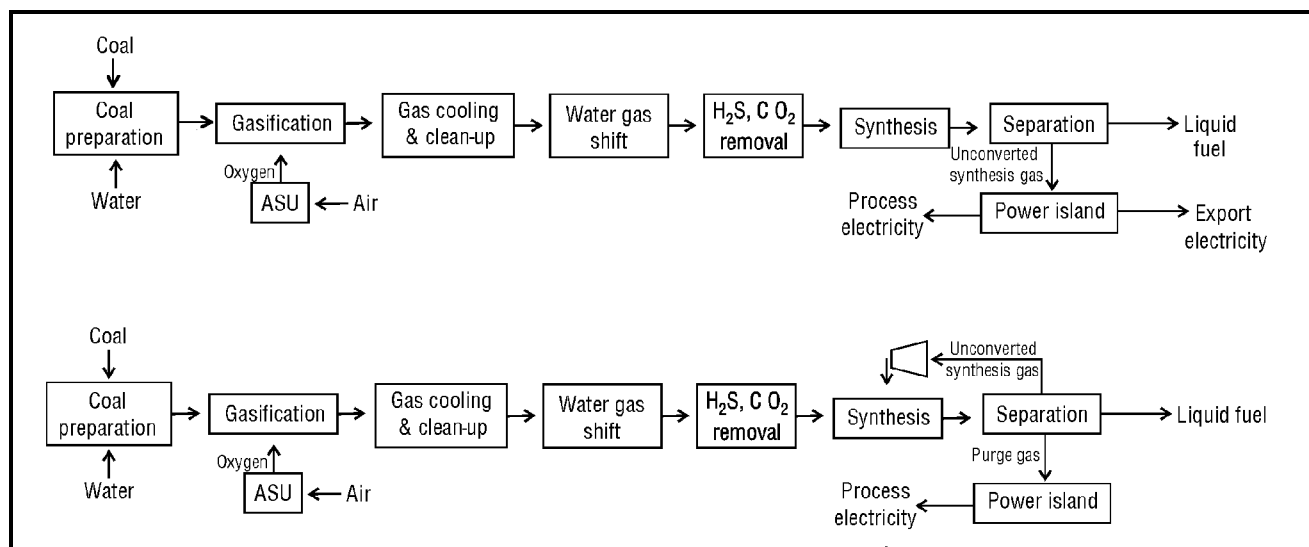


Figure 1. Two basic process configurations for liquid fuel production by indirect coal liquefaction: upper, “once-through” synthesis with exportable electricity co-product; lower, “recycle” synthesis with no net exportable electricity production

Table 1. Properties of dimethyl ether, propane, and petroleum diesel

	Dimethyl ether	Propane	Petroleum diesel
Boiling temperature, °C	-24.9	-42.1	180-370
Vapor pressure, atmospheres	5.1	8.4	<< 1
Liquid density, kg/m <sup>3</sup>	668	501	~840
Liquid lower heating value, MJ/kg	28.4	46.0	42.5
Flammability limits in air, vol %	3.4-17	2.1-9.4	0.6-6.5
Auto-ignition temperature, °C	235	470	250
Cetane number	55-60	5	40-55

bonds, and NO<sub>x</sub> emissions are lower than when using conventional diesel fuel [Fleisch et al., 1997; Zhou et al., 2000; Fleisch et al., 1995; Sorenson and Mikkelsen, 1995]. DME can be reformed into hydrogen at least as easily as methanol, and thus is potentially suitable for future use as a hydrogen source for stationary or vehicle fuel cells. One drawback of DME as a vehicle fuel is the need for modest pressurization to store it as a liquid (Table 1). DME can also be used as an LPG substitute in domestic applications, e.g., cooking, where it burns with a clean blue flame over a wide range of air/fuel ratios [Fleisch et al., 1995; ICC, 2003]. DME is relatively inert, non-corrosive, non-carcinogenic, almost non-toxic, and does not form peroxides by prolonged exposure to air [Hansen et al., 1995].

DME is produced globally today at a rate of about 150,000 tonnes (t) per year in small-scale facilities by dehydration of MeOH [Naqvi, 2002]. Technologies are available for converting syngas from natural gas or coal directly into DME (rather than with intermediate methanol production), but the small size of today’s DME markets has not justified building direct conversion facilities, which require relatively large scale to achieve attractive economics. The Chinese Ningxia coal-to-DME project has a planned output capacity of 830,000 t/yr DME using a direct conversion process, and the principal intended

application is as a household cooking fuel [Lucas, 2002].

In this paper, we present detailed process designs and performance estimates for production of DME from coal, together with cost analysis. Since there are many similarities to methanol production, which is more widely understood, we include self-consistent analyses of methanol from coal for reference.

## 2. Basic process configurations for indirect coal liquefaction

Figure 1 illustrates two basic process configurations for making MeOH, DME, or Fischer-Tropsch fuels by indirect coal liquefaction. The difference between the two is that in one case the only output from the facility is a liquid fuel. In the other case, electricity is a major co-product. The two configurations are essentially identical through the first few process steps.

The first process step is gasification, which converts the coal into a “synthesis gas” (or syngas) containing primarily hydrogen (H<sub>2</sub>) and carbon monoxide (CO). A variety of gasifier designs are in commercial operation worldwide using coal or other dirty, low-value feedstocks (e.g., petroleum coke generated at refineries) [Simbeck and Johnson, 2001]. Here we have chosen to consider a design based on the technology of Chevron/Texaco. This design uses partial oxidation of the coal in oxygen (generated in a dedicated air separation unit) to provide the requisite heat to drive the gasification reactions. The coal is fed into the reactor in a water slurry, which has two important implications. Feeding can be done into a vessel operating at relatively high pressures (75 bar in plant configurations considered in this paper), which provide thermodynamic and cost benefits to the overall process, and the additional hydrogen (in the slurry water) promotes a larger H<sub>2</sub> fraction in the syngas compared to a dry-feed gasifier design.

Following gasification, the raw syngas is cooled and cleaned of contaminants. Two approaches for the initial cooling step are the use of a direct water quench or a

high-temperature syngas cooler. Either of these would be followed by a wet scrubbing step to remove fine particles. A water-gas shift (WGS) reactor is incorporated after the initial cooling to adjust the ratio of H<sub>2</sub> to CO in the syngas to give an optimal ratio for subsequent downstream chemical processing. Sulfur-tolerant water-gas shift catalysts are available (e.g., a CoMo catalyst made by Haldor Topsoe [2002]), so that sulfur removal (which is necessary to protect further-downstream catalysts) can be done after the shift. Additional steam may be added to the shift reactor to ensure a sufficient steam-carbon ratio to avoid coke formation [Katofsky, 1993]. Before the sulfur removal step, an inexpensive activated carbon filter would be used to capture trace contaminants such as mercury and other heavy metals [Rutkowski et al., 2002].

The sulfur removal step is critical, both to limit SO<sub>2</sub> emissions from the conversion facility (e.g., in the case where some of the syngas is burned in a gas turbine) and to protect the catalysts used in the downstream synthesis step. The latter requirement places a stricter constraint on sulfur removal than the former [Turk et al., 2001]. Sulfur levels below 1 ppmv in the synthesis feed gas are required to guarantee adequate catalyst life [Moore, 2003]. Several technologies are commercially available that can achieve such levels, including those that operate using physical absorption into organic fluids (e.g., Selexol<sup>®</sup> or Rectisol<sup>®</sup>) and others that operate by chemical reaction of amines with the sulfur compounds in the gas.

Unlike chemical absorption processes, the effectiveness of physical absorption processes is proportional to the partial pressure of the gases to be removed (e.g., H<sub>2</sub>S). Since the syngas is available at elevated pressure (> 60 bar) in the systems considered here, physical absorption is the preferred sulfur removal technology. The characteristics and costs of Selexol<sup>®</sup> technology, which in typical applications (e.g., sulfur removal from syngas for gas turbine combustion) achieves H<sub>2</sub>S concentrations down to 20 ppmv, but which can also achieve H<sub>2</sub>S removal to the 1 ppm level [Sharp et al., 2002], are the basis for the H<sub>2</sub>S removal designs here. The captured H<sub>2</sub>S is typically converted to elemental sulfur using the Claus process, with tail gas clean-up in a SCOT plant. Following the Selexol unit, a final sulfur guard bed (e.g. using zinc-oxide bed material) is used to remove residual H<sub>2</sub>S to ppb levels.

Selexol solvent absorbs CO<sub>2</sub> in addition to H<sub>2</sub>S. (The solubility of CO<sub>2</sub> in Selexol is about one-ninth that of H<sub>2</sub>S [Breckenridge et al., 2000].) In theory, the removal of all CO<sub>2</sub> (along with the H<sub>2</sub>S) is desirable to maximize downstream synthesis to methanol or DME (as discussed in Section 3.1 below), but in practice some CO<sub>2</sub> is required in the gas to provide oxygen needed to maintain the activity of the synthesis catalyst<sup>[3]</sup>. The CO<sub>2</sub> may be vented, captured for sale as a by-product, or captured for below-ground storage. The idea of co-capture and co-storage of H<sub>2</sub>S and CO<sub>2</sub> has also been proposed [Chiesa et al., 2003]. This would have significant cost advantages for coping with sulfur, since no Claus/SCOT plant would be needed to convert the H<sub>2</sub>S into elemental sulfur, and separate systems for desorbing H<sub>2</sub>S and CO<sub>2</sub> from the

Selexol solvent would not be needed.

The clean syngas leaving the sulfur removal area is sent to the synthesis area of the plant. The gas is preheated to the operating temperature of the synthesis reactor (~260°C) before being fed into it. In a single pass of gas through the synthesis reactor, only a portion of the CO and H<sub>2</sub> will be converted to the desired liquid fuel. After synthesis, purification of the raw synthesis product by a series of flash tanks and/or distillation steps produces the final liquid fuel of interest.

In one of the basic plant configurations considered here (Figure 1, upper) the syngas is passed only once through the synthesis reactor (“once-through” configuration). The unconverted gas is used as fuel for a gas turbine. The hot exhaust of the turbine is used, together with waste heat recovered from various places in the process, to raise steam to drive a steam turbine. The power generated by the gas turbine/steam turbine combined cycle is sufficient to provide the power needed to operate the plant, plus a significant amount of power for export to the grid.

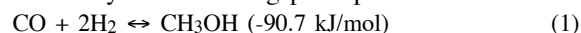
In the other basic plant configuration (Figure 1, lower), most of the unconverted gas from the product recovery area is returned to the synthesis reactor to generate additional liquid fuel (“recycle” configuration). The remainder of the unconverted gas fuels a power cycle making only enough power to meet the process needs, with no additional electricity for export.

### 3. DME synthesis chemistry and technology

Process technologies for producing a clean synthesis gas from coal are relatively well established commercially [Simbeck and Johnson, 2001]. Methanol production from a synthesis gas is also a relatively well-established technology, but DME synthesis is a relatively less well-known process, which motivates the discussion in this section.

#### 3.1. Chemistry of dimethyl ether synthesis

The synthesis of methanol from syngas is typically carried out over a catalyst (e.g., CuO/ZnO/Al<sub>2</sub>O<sub>3</sub>) and can be characterized by the following principal reaction.



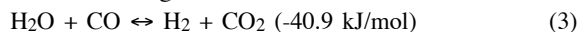
As noted earlier, commercial processes for making DME today involve dewatering methanol over a dehydration catalyst (e.g.,  $\gamma$ -alumina) as a separate step from methanol production.



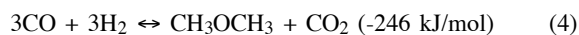
By combining some methanol catalyst and dehydration catalyst in the same reactor, Reactions (1) and (2) proceed simultaneously, resulting in direct synthesis of DME. The idea of direct synthesis of DME from syngas was first reported in the literature long ago [Brown and Galloway, 1929], but efforts to commercialize direct synthesis technology did not begin in earnest until around 1990. The renewed work on direct DME synthesis originated, in part, from an interest in finding ways to increase the conversion of syngas to a liquid fuel beyond the conversion achievable for methanol [Sofianos and Scurrill, 1991].

Syngas conversion to methanol (Equation 1) can be accomplished today to nearly the extent predicted by chemical equilibrium, i.e., the syngas is converted to methanol

at essentially the theoretical maximum rate. Substituting methanol dehydration catalyst for some of the methanol synthesis catalyst in a one-step DME synthesis reactor results in methanol being reacted away (by Equation 2) as it forms. This effectively by-passes the equilibrium limits of Equation 1. Furthermore, when the syngas is rich in CO (as from coal gasification) the methanol catalyst also promotes the water-gas shift reaction.



This provides a further synergistic effect, whereby the water that forms during dehydration (which would otherwise limit the extent of Equation 2) drives  $\text{H}_2$  production, which in turn drives additional methanol production by Equation 1. The entire single-step DME synthesis chemistry can be represented as a combination of Equations 1, 2, and 3:



In this case, the optimum ratio between  $\text{H}_2$  and CO in the feed gas to a synthesis reactor is 1, compared to a value of 2 for methanol synthesis (Equation 1).

### 3.2. Synthesis reactor design considerations

Because the synthesis of methanol or DME is exothermic (see Equation 4), the temperature in a synthesis reactor will rise as the reactions proceed if no heat is removed. Higher temperatures promote faster reaction, but reaching equilibrium (i.e., maximum) conversion levels is favored by lower temperatures, and catalysts are deactivated when overheated. Thus, the temperature rise in a synthesis reactor must be controlled. In practice, a reactor operating temperature of 250–280°C balances kinetic, equilibrium, and catalyst activity considerations.

Two available synthesis reactor designs, gas-phase (or fixed-bed) and liquid-phase (or slurry-reactor), handle temperature control using different approaches. The basic gas-phase design involves the flow of syngas over a fixed bed of catalyst pellets. The basic liquid-phase design involves bubbling syngas through an inert mineral oil containing powdered catalyst in suspension.

In a gas-phase reactor, it is difficult to maintain isothermal conditions by direct heat exchange (because of low gas-phase heat transfer coefficients). To limit temperature rise, the synthesis reactions are staged, with cooling between reactor stages. Also, by limiting the initial concentration of CO entering the reactor (to 10–15 vol %) the extent of the exothermic reactions can be controlled. Control of the CO fraction is achieved in practice by maintaining a sufficiently high recycling of unconverted  $\text{H}_2$ -rich syngas back to the reactor.

The Haldor Topsoe fixed-bed system design includes three stages of synthesis reactors with cooling between each stage and recycling of unconverted syngas [Hansen et al., 1995]. The patent for this process specifies a feed gas CO concentration of less than 10 % and a recycled volume of unconverted syngas ranging from 93 % to 98 % of the total unconverted syngas [Voss et al., 1999]. The fraction of CO converted on a single pass through each reactor stage (assuming a three-stage intercooled set of reactors) ranges from 16 % to 34 %, depending on the  $\text{H}_2/\text{CO}$  ratio.

In a liquid-phase reactor, the inert fluid moderates the temperature rise and also allows for more effective heat transfer to boiler tubes immersed in the fluid. Much higher heat release rates can be accommodated without excessive temperature rise than in a gas-phase reactor. Best advantage of the good temperature control can be taken with CO-rich syngas [Peng et al., 1999a], such as that produced by coal gasification. With such feed gases, high conversion of CO is possible in a single pass of the gas through a relatively small reactor.

The leading commercial developer of fixed-bed DME synthesis reactor designs is Haldor Topsoe [Hansen et al., 1995; Voss et al., 1999]. Mobil and Snamprogetti S.p.A. hold patents for DME synthesis processes [Zahner, 1977; Pagani, 1978], but at present are not pursuing commercial development of the technology. Leading private developers of slurry-bed DME synthesis reactors are Air Products and Chemicals, Inc. (APCI) [Brown et al., 1991; Lewnard et al., 1993; Peng et al., 1999a; Peng et al., 1999b; Lewnard et al., 1990] and the NKK Corporation [Adachi et al., 2000; Fujimoto et al., 1995]. The Institute of Coal Chemistry of the Chinese Academy of Sciences (Taiyuan) [Niu, 2000] has also been developing slurry-phase DME synthesis technology since 1995. The CAS Institute of Chemical Physics (Dalian) has done some work on fixed-bed DME synthesis technology [Xu et al., 2001]. Researchers at Zhejiang University (in Hangzhou) and at the East China University of Science and Technology (Shanghai) are also involved in DME-related work.

The DME reactor design of APCI is derived from its liquid-phase methanol (LPMEOH) synthesis process that was developed in the 1980s with the support of the US Department of Energy. A commercial-scale LPMEOH demonstration plant (250 tonnes per day (t/d) methanol capacity) has been operating since 1997 with gas produced by the Eastman Chemical Company's coal gasification facility in Kingsport, Tennessee [Eastman, 2003]. The construction of this facility was preceded by extensive testing in a 10 t/d capacity process development unit (PDU) in LaPorte, Texas. The PDU was operated in 1999 to generate test data on direct DME synthesis [Air Products, 2001; Air Products, 2002].

DME Development, Inc., a Japanese consortium of nine companies led by NKK and Nippon Sanso, is currently in the design/build stage for a 100 t/d DME slurry-phase reactor planned for testing during 2004–2006 in Kushiro, Hokkaido. This effort builds on initial testing of a 5 t/d capacity reactor that was completed in 1999 by NKK [2003], which before that (with support from the Japanese Ministry of International Trade and Industry) worked with the Taiheiyo Coal Mining Co., Sumitomo Metal Industries, and Japan's Center for Coal Utilization to develop the DME slurry reactor technology.

## 4. Process modeling of methanol and DME production by ICL

With the objective of better understanding system design and cost trade-offs for ICL processes, we used AspenPlus chemical process simulation software to calculate detailed

mass and energy balances for a variety of ICL configurations. This section summarizes our modeling approach and validation efforts for gasification, synthesis, power generation, and overall process heat integration.

The gasifier performance significantly affects the performance of the overall process, so accurate gasifier simulation is essential. Because reaction temperatures in coal gasifiers are relatively high, a chemical equilibrium-based simulation will accurately predict product gas composition. We have based our analyses on Chevron/Texaco gasification technology, but our modeling approach can also be used for other gasifier designs and arbitrary coal types. The differences between heat and material balances predicted using our model and those reported elsewhere [SFA Pacific, 1993] are small for the parameters that are most important in predicting overall ICL process performance, namely the amount of CO and H<sub>2</sub> produced and the gasifier cold-gas efficiency (Table 2).

For the synthesis reactor, it is possible to use a chemical equilibrium-based simulation for methanol [Katofsky, 1993] or DME synthesis [Gogate and Vijayaraghavan, 1992], but such models are less flexible in simulating alternative operating conditions (e.g., different reactor space velocities, or, in the case of DME, the effect of different mass ratios of methanol synthesis catalyst to dehydration catalyst). We chose instead to develop self-consistent kinetic models for methanol synthesis and DME synthesis. One drawback of this approach is that kinetic data in the open literature are not in complete agreement [Natta, 1955; Leonov et al., 1973; Cybulsky, 1994; Dybkjaer, 1985; Chinchin et al., 1984; Graaf et al., 1988a; Vanden Bussche and Froment, 1996; Klier et al., 1982].

After a thorough literature review, we chose to use kinetic rate equations for methanol synthesis developed by Graaf [Graaf et al., 1988b; Graaf and Beenackers, 1996] from laboratory measurements with a batch liquid-phase reactor and a CuO/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst. Among the rate equations in the literature for which complete information was provided by authors, Graaf's equations appear to be relatively conservative in their prediction of the fractional conversion of CO to methanol. For the DME synthesis model, we added to these reactions a kinetic expression for methanol dehydration (over a  $\gamma$ -alumina catalyst) developed by Ng et al. [1999].

In all of the results reported here, we used a gas space velocity of 6000 l/hr·kg<sub>cat</sub> (standard liters input syngas per hour per kilogram of methanol synthesis catalyst). For all DME cases, we used a mass ratio of methanol dehydration catalyst to methanol synthesis catalyst of 0.3. With these parameter values, our synthesis reactor performance predictions compare well with the predictions of synthesis models developed for internal use by Air Products and Chemicals, Inc. [Moore, 2003]. The APCI predictions against which our results were compared were based on typical lifecycle reactor performance, including an assumed catalyst activity level of 50 % of the level for fresh catalyst.

The power island in our simulations was based on a gas turbine/steam turbine combined cycle<sup>[4]</sup>. The gas tur-

bine burns unconverted syngas in the "once-through" process designs. In the recycle cases, recycle purge gas is augmented as fuel by a minor amount of syngas that bypasses the synthesis reactor. In the once-through cases, the power island was sized to use all of the available unconverted syngas. In the recycle cases, it was sized to generate sufficient power to meet all or most of the process electricity requirements with little or no electricity available for export.

The gas turbine was modeled on the most advanced generation of operating machines now available on the market ("F" technology). We calibrated our performance predictions against results from gas turbine simulation software of the Politecnico di Milano (Italy), the accuracy of which has been extensively demonstrated in earlier work [Chiesa et al., 2003; Consonni, 1992; Chiesa and Macchi, 2002].

Heat in the exhaust flow of the gas turbine is recovered in a heat recovery steam generator (HRSG) generating steam at high pressure (165 bar), medium pressure (38 bar), and low pressure (7 or 4 bar). Heat recovered elsewhere in the process (e.g., medium-pressure steam generated by cooling of the synthesis reactor) is also integrated into the HRSG. The design of the heat exchange network for low-pressure steam generation from process waste heat streams was optimized using pinch analysis, a well-established method for optimizing the energy performance of industrial processes [Linnhoff, 1993]. All steam from the HRSG is expanded through a condensing steam turbine (0.05 bar condenser pressure) to generate electricity.

## 5. Process simulation results

Using the modeling approach described above, we developed several alternative process designs for methanol and for DME production, with and without co-production of exportable electricity. All of our analyses were done for a representative bituminous coal from the area of Yanzhou City in Shandong Province, China (Table 3).

### 5.1. Methanol production

Process designs with "once-through" (OT) synthesis and with "recycle" (RC) synthesis were developed for methanol from coal. Detailed material balances for each design are described in the next sections, followed by a summary comparison of performances.

#### 5.1.1. With once-through synthesis design – OT

Figure 2 and the upper section of Table 4 describe the detailed material balance for the OT plant design for methanol. In this design, the feed coal (3992 t/d, as-received) is mixed with water to form a slurry that is pumped into a Texaco-type gasifier operating at 75 bar pressure and reaching 1390°C operating temperature. Oxidant with a purity of 94.3 % O<sub>2</sub> is supplied to the gasifier from a dedicated air separation unit. In the lower section of the gasifier, the raw synthesis gas passes through a quench, followed by an external scrubber that removes any remaining particulate matter. The gas leaves the scrubber at 246°C with an H<sub>2</sub>/CO ratio of 0.62 (Table 4).

After the scrubber, some of the raw synthesis gas passes

Table 2. Comparison of reference<sup>[1]</sup> and calculated performance of alternative gasifier designs

Gasifier design		Texaco	Shell	Shell	Destec				
<b>Inputs</b>									
<b>Coal type</b>		<b>IL no. 6 bituminous</b>	<b>IL no. 6 bituminous</b>	<b>Texas lignite</b>	<b>Texas lignite</b>				
Coal ultimate analysis (dry wt %)	Ash	9.90	18.15	16.58	16.59				
	C	69.58	65.33	60.92	60.83				
	H	5.31	4.17	4.42	4.45				
	N	1.26	1.06	1.08	1.08				
	Cl	0.09	0.08	0.08	0.15				
	S	3.87	4.58	1.08	1.08				
	O	9.99	6.62	15.83	15.82				
Moisture (wet wt %)		12.03	2.47	4.46	34.90				
Coal feed	kg/s	9.5	9.48	9.5	13.9				
	bar	42.4	25.13	28.6	28.6				
	°C	121.1	80.00	80.0	80.0				
	HHV, J/g dry	29708	26683	24364	24367				
Slurry water	kg/s	3.08	0.43	0.00	4.20				
	bar	42.4	43.4	1.0	28.6				
	°C	121.1	343.3	0.0	80.0				
Nitrogen	kg/s	0.00	0.70	0.70	0.00				
	bar	1.0	25.1	28.6	1.0				
	°C	0.0	80.0	80.0	0.0				
Oxidant	mol % O <sub>2</sub>	94.30	94.33	94.34	94.31				
	mol % Ar	4.52	4.48	4.51	4.52				
	mol % N <sub>2</sub>	1.18	1.19	1.16	1.17				
	kg/s	7.7	7.60	6.5	8.1				
	bar	47.0	25.14	28.6	30.0				
	°C	83.3	120.00	120.0	120.0				
Gasification temp, °C		1371.1	1426.70	1371.1	1037.8				
<b>Reference values and calculated outputs</b>									
		<b>Ref</b>	<b>Calc</b>	<b>Ref</b>	<b>Calc</b>	<b>Ref</b>	<b>Calc</b>	<b>Ref</b>	<b>Calc</b>
Gasifier output (clean syngas)	mol % CO	39.61	41.75	63.06	63.49	60.65	61.26	21.83	21.48
	mol % H <sub>2</sub>	30.31	28.33	26.75	26.39	27.58	27.41	24.62	24.37
	mol % CO <sub>2</sub>	10.79	8.56	1.49	1.18	2.76	2.16	17.16	17.14
	mol % H <sub>2</sub> O	16.47	18.44	2.01	1.67	3.21	3.07	34.67	35.11
	mol % CH <sub>4</sub>	0.08	0.01	0.03	0.07	0.03	0.07	0.03	0.09
	mol % Ar	0.91	1.13	1.10	1.37	1.03	1.26	0.78	0.97
	mol % N <sub>2</sub>	0.73	0.69	4.08	4.08	4.34	4.30	0.54	0.55
	mol % H <sub>2</sub> S	1.00	1.00	1.30	1.56	0.32	0.39	0.25	0.25
	mol % COS	0.03	0.07	0.14	0.17	0.04	0.04	0.01	0.01
	kmol/s	0.953	0.951	0.773	0.765	0.719	0.717	1.174	1.172
kg/s	19.43	19.39	16.50	16.43	15.19	15.14	24.68	24.64	
Heat loss, % of coal HHV <sup>[2]</sup>		N/A <sup>[3]</sup>	0.33	N/A <sup>[3]</sup>	2.72	N/A <sup>[3]</sup>	1.85	N/A <sup>[3]</sup>	1.15
Cold-gas efficiency (HHV %)		76.3%	76.1%	80.0%	79.4%	81.8%	82.0%	70.6%	69.9%
Calc / ref efficiencies		0.997		0.992		1.003		0.989	

**Notes**

1. The upper section of this table (Inputs) and the Ref values in the lower section are from SFA Pacific [1993].
2. In our calculated results, heat loss was adjusted to match the calculated gasification temperature with the published value.
3. N/A = Not available.

to an adiabatic WGS reactor (called a “sour” WGS because of its sulfur-tolerant catalyst). Heat released during the WGS reaction is largely recovered from the exit gases as steam, which is injected into the WGS reactor to ensure effective performance. The shifted gas rejoins the portion of the syngas that bypassed the WGS. At this point, the

H<sub>2</sub>/CO ratio of the synthesis gas is 2 – essentially the optimum ratio for methanol synthesis.

The gas also contains sulfur, primarily as hydrogen sulfide (H<sub>2</sub>S), but also with some carbonyl sulfide (COS). A COS hydrolysis unit is used to convert COS to H<sub>2</sub>S, the latter being a more readily removable form of sulfur.

The hydrolysis unit is followed by heat exchangers that cool the gas to the temperature required by the acid gas removal system (AGR). As discussed earlier, the AGR removes H<sub>2</sub>S to the low level required by the synthesis reactor, and it is also designed to remove the bulk of the CO<sub>2</sub>. Some CO<sub>2</sub> is left in the gas to ensure good synthesis catalyst activity.

Following the AGR, the gas at 70 bar is heated to nearly 250°C using the product stream from the synthesis reactor and then fed to the reactor. Steam generated in boiler tubes immersed in the liquid reactor bed maintains essentially isothermal synthesis conditions (260°C). The mixture of gases leaving the reactor passes to the product separation area, where a series of flash tanks separates methanol from unconverted synthesis gas. In the product

**Table 3. Coal composition for process simulations (representative of Yanzhou, Shandong Province, China)**

As-received	
Moisture (wt %)	7.11
HHV(MJ/kg)	24.536
LHV (MJ/kg)	23.494
Ultimate analysis (dry wt %)	
Ash	20.23
C	63.67
H	4.28
O	6.75
S	3.97
N	1.09
Cl	0.01

**Table 4. Material balances for once-through and recycle methanol-from-coal processes**

	Scrubber exit	Water gas shift reactor, inlet	Water gas shift reactor, exit	H <sub>2</sub> S removal unit, inlet	H <sub>2</sub> S removal unit, exit	Total feed into synthesis (inc. recy.)	Recycle gas feed into synthesis	Raw synthesis product	Final liquid product	Fuel gas to gas turbine
<b>Methanol: once-through synthesis</b>										
Figure 2 stream no.	11	13	14	19	22	23		25	27	28
kg/s	177.90	86.75	100.86	95.41	37.87	37.87	-	37.87	12.69	28.19
kmol/s	9.170	4.471	5.255	4.591	3.156	3.156	-	2.356	0.395	2.129
mol fraction										
CO	0.2021	0.2021	0.0100	0.2183	0.3176	0.3176	-	0.2552	0.0021	0.2820
H <sub>2</sub>	0.1258	0.1258	0.2690	0.4366	0.6351	0.6351	-	0.5116	0.0000	0.5663
CO <sub>2</sub>	0.0430	0.0430	0.1986	0.2720	0.0198	0.0198	-	0.0269	0.0126	0.0275
H <sub>2</sub> O	0.6143	0.6143	0.5098	0.0434	0.0013	0.0013	-	0.0013	0.0020	0.0796
O <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-	0.0000	0.0000	0.0000
N <sub>2</sub>	0.0033	0.0033	0.0028	0.0065	0.0095	0.0095	-	0.0127	0.0001	0.0140
Ar	0.0057	0.0057	0.0048	0.0113	0.0164	0.0164	-	0.0220	0.0002	0.0243
CH <sub>4</sub>	0.0001	0.0001	0.0001	0.0002	0.0003	0.0003	-	0.0004	0.0000	0.0004
H <sub>2</sub> S	0.0054	0.0054	0.0046	0.0116	0.0000	-	-	-	-	-
COS	0.0004	0.0004	0.0003	0.0000	0.0000	-	-	-	-	-
CH <sub>3</sub> OH	-	-	-	-	-	-	-	0.1698	0.9828	0.0058
CH <sub>3</sub> OCH <sub>3</sub>	-	-	-	-	-	-	-	-	-	-
<b>Methanol: recycle synthesis</b>										
Figure 3 stream no.	11	13	14	19	22+23	25	29	27	30	32
kg/s	175.50	84.67	97.97	92.86	33.92	166.36	132.62	166.36	32.03	2.0822
kmol/s	9.108	4.394	5.133	4.521	3.057	11.296	8.253	9.327	0.997	0.1037
mol fraction										
CO	0.2039	0.2039	0.0105	0.2245	0.3320	0.2680	0.2445	0.2189	0.0013	0.2684
H <sub>2</sub>	0.1271	0.1271	0.2728	0.4422	0.6539	0.5342	0.4901	0.4361	0.0000	0.3202
CO <sub>2</sub>	0.0429	0.0429	0.2008	0.2734	0.0052	0.0201	0.0257	0.0246	0.0105	0.0687
H <sub>2</sub> O	0.6178	0.6178	0.5087	0.0430	0.0013	0.0011	0.0010	0.0011	0.0018	0.1111
O <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N <sub>2</sub>	0.0020	0.0020	0.0017	0.0040	0.0060	0.1410	0.1908	0.1707	0.0009	0.1670
Ar	0.0004	0.0004	0.0004	0.0008	0.0012	0.0270	0.0364	0.0327	0.0002	0.0343
CH <sub>4</sub>	0.0001	0.0001	0.0001	0.0002	0.0003	0.0040	0.0054	0.0049	0.0002	0.0075
H <sub>2</sub> S	0.0054	0.0054	0.0047	0.0118	0.0000	-	-	-	-	-
COS	0.0004	0.0004	0.0003	0.0000	0.0000	-	-	-	-	-
CH <sub>3</sub> OH	-	-	-	-	-	0.0044	0.0061	0.1109	0.9848	0.0224
CH <sub>3</sub> OCH <sub>3</sub>	-	-	-	-	-	-	-	-	-	-

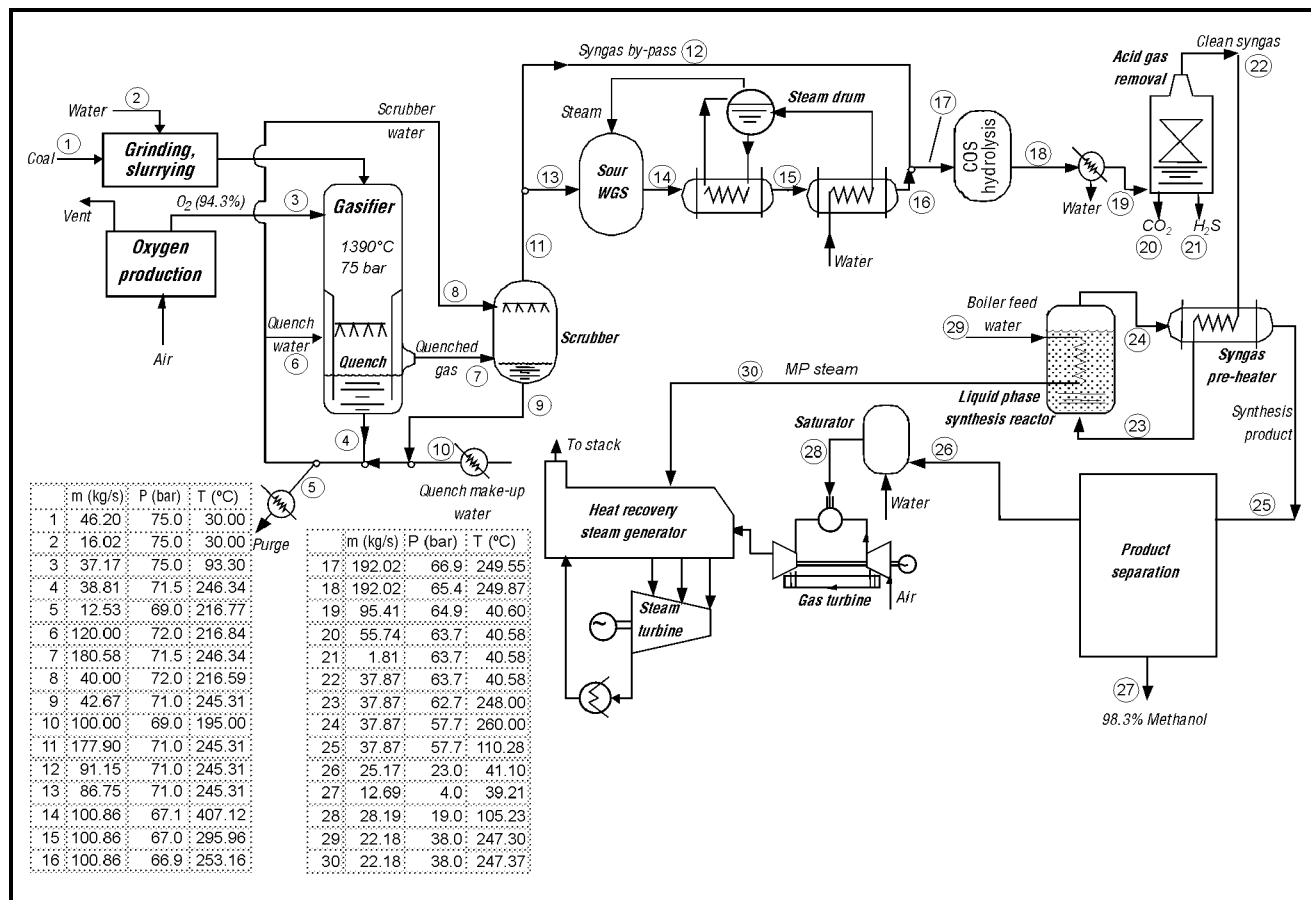


Figure 2. Methanol and electricity from coal based on “once-through” liquid-phase synthesis

separation area, a syngas expander reduces the pressure of the unconverted syngas and generates some electricity.

Unconverted synthesis gas from product separation is humidified and then burned in a gas turbine/steam turbine combined cycle to generate electricity, a portion of which is required to run the whole process. Heat recovered from the synthesis reactor and various other points in the process augments steam production in the heat recovery steam generator of the combined cycle island.

5.1.2. With recycle synthesis design – RC

In the recycle design, the only exported product is methanol; electricity is generated within the plant, but only to meet electricity needs for the process. The process configuration (Figure 3 and Table 4, lower) is similar to the OT design, with three major differences. Most importantly, the unconverted synthesis gas recovered in the product separation area is compressed and recycled back to the synthesis reactor. Second, the purity of the oxidant supplied to the gasifier is increased to 99.5 % O<sub>2</sub> to avoid excessive build-up of inert gases in the synthesis recycle loop. Also, the power island is based on a steam-Rankine cycle rather than a combined cycle, as noted earlier<sup>[4]</sup>.

5.1.3. Methanol performance summary

Table 5 summarizes the mass and energy balances for the two basic process configurations described above, all of which are sized to the same coal input rate (3992 t/d). Additionally, three sub-cases are shown for each of the two designs. The sub-cases differ from each other in how the H<sub>2</sub>S and CO<sub>2</sub> removed at the AGR are subsequently

handled. In the sub-case labeled “vent”, the captured H<sub>2</sub>S is converted to elemental sulfur and the CO<sub>2</sub> is vented to the atmosphere. In the case labeled “capture”, the H<sub>2</sub>S is converted to elemental sulfur and most of the CO<sub>2</sub> is separately dried and compressed to 150 bar for pipeline distribution to an injection site for long-term below-ground storage. (A small amount of CO<sub>2</sub> originally removed from the synthesis gas in the AGR would be unavoidably vented to the atmosphere in this case.) In the case labeled “co-capture”, all of the H<sub>2</sub>S and CO<sub>2</sub> removed at the AGR are dried and compressed together for pipeline shipment to an underground storage site.

In the OT plant design with CO<sub>2</sub> venting, 23 % of the energy input as coal is converted to methanol (247 MW<sub>LHV</sub>), with an equivalent fraction converted to exportable electricity (247 MW<sub>e</sub>). By comparison, the RC plant design with CO<sub>2</sub> venting produces 626 MW of methanol (58 % of coal energy input), but very little exportable electricity. With CO<sub>2</sub> capture and storage, the OT designs produce the same amount of methanol as with CO<sub>2</sub> venting, but electricity output is reduced slightly due to on-site electricity requirements for drying and compressing CO<sub>2</sub> (or CO<sub>2</sub> plus H<sub>2</sub>S) for transport to an underground storage site. The RC designs with CO<sub>2</sub> capture also maintain the same methanol output as with CO<sub>2</sub> venting, but some electricity must be imported to the plant to meet on-site electricity demands.

For comparison with other liquid fuel production systems, the effective efficiency of methanol production can

Table 5. Methanol summary mass and energy balances with same coal input for all cases

Management of captured CO <sub>2</sub>	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
<b>Coal feed rate</b>						
As-received t/d	3992	3992	3992	3992	3992	3992
Dry t/d	3708	3708	3708	3708	3708	3708
Moisture and ash free (MAF) t/d	2958	2958	2958	2958	2958	2958
MW HHV	1134	1134	1134	1134	1134	1134
MW LHV	1085	1085	1085	1085	1085	1085
Carbon in coal, kgC/GJ LHV	25.2	25.2	25.2	25.2	25.2	25.2
<b>Oxygen feed rate</b>						
Total oxidant, t/d	3214	3214	3214	3007	3007	3007
Oxidant purity (mol % O <sub>2</sub> )	94.3 %	94.3 %	94.3 %	99.5 %	99.5 %	99.5 %
Pure O <sub>2</sub> , t/d	3032	3032	3032	2992	2992	2992
<b>Carbon dioxide</b>						
Removed from syngas, tCO <sub>2</sub> /d	4511	4511	4511	4639	4639	4639
Captured for storage, tCO <sub>2</sub> /d	0	4157	4511	0	4286	4639
<b>Methanol product</b>						
Total product output, t/d	1096	1096	1096	2768	2768	2768
Product purity (mol % methanol)	98.28	98.28	98.28	98.48	98.48	98.48
MW HHV	281.7	281.7	281.7	713.2	713.2	713.2
MW LHV	247.3	247.3	247.3	626.0	626.0	626.0
MW output relative to recycle (scale factor)	2.53	2.53	2.53	1.00	1.00	1.00
<b>Electricity</b>						
<b>Gross production (MW)</b>						
Gas turbine	174.5	174.5	174.5	0	0	0
Steam turbine	125.2	125.2	125.2	63.1	63.1	63.1
Syngas expander	0	0	0	0	0	0
Total gross production	299.7	299.7	299.7	63.1	63.1	63.1
<b>On-site consumption (MW)</b>						
Air separation unit <sup>[1]</sup>	50.20	50.20	50.20	48.90	48.90	48.90
Recycle compressor	0.00	0.00	0.00	4.4	4.40	4.40
Synthesis island	0.43	0.43	0.43	1.91	1.91	1.91
Product separation	0.07	0.07	0.07	0.27	0.27	0.27
CO <sub>2</sub> drying/compression <sup>[2]</sup>	0.00	16.94	18.97	0	17.46	19.50
Balance of plant	2.00	2.00	2.00	2.50	2.50	2.50
Total on-site consumption	52.70	69.64	71.68	57.97	75.43	77.47
<b>Total net sales to grid (MW)</b>	247.0	230.1	228.0	5.1	-12.3	-14.4
<b>Fraction of coal LHV converted to</b>						
Methanol	0.228	0.228	0.228	0.577	0.577	0.577
Exportable electricity	0.228	0.212	0.210	0.005	-0.011	-0.013
Methanol + electricity	0.455	0.440	0.438	0.581	0.565	0.564
<b>Plant carbon flows (at 85 % capacity factor)</b>						
Input coal, ktC/yr <sup>[3]</sup>	732	732	732	732	732	732
Captured/stored, ktC/yr	0	352	382	0	363	393
In methanol product, ktC/yr	125	125	125	316	316	316
Emissions at plant, kt/yr	608	256	226	416	53	24
<b>Effective methanol efficiency<sup>[4]</sup></b>	48.4	45.0	44.6	58.3	56.2	56.0

## Notes

- Air separation was not modeled explicitly. Electricity consumption of 390 kWh/t of oxidant was assumed for 99.5 % purity oxidant and 375 kWh/t for 94.3 % purity oxidant.
- CO<sub>2</sub> drying and compression was not modeled explicitly. Electricity consumption of 97.8 kWh/tCO<sub>2</sub> (or 97.8 kWh/t(CO<sub>2</sub>+H<sub>2</sub>S)) was assumed [Chiesa et al., 2003].
- This is carbon carried into the plant with the coal. Upstream carbon emissions (associated with coal-mining and delivery to the plant) are not included in this number. Upstream emissions are estimated to be 1 kgC/GJ of delivered coal (LHV basis) [Ogden et al., 2004], or 29 ktC/yr (85 % capacity factor) for the plants in this table.
- The effective efficiency is defined as F/(C-E/N), where F is the output of fuel DME (LHV MW), C is the total coal input (LHV MW), E is the exportable electricity production (MW), and N is the efficiency of electricity production from coal (LHV basis) in a stand-alone power plant. In this calculation, the stand-alone power plant is assumed to be an IGCC plant for which N is 43 % [Chiesa et al., 2003].

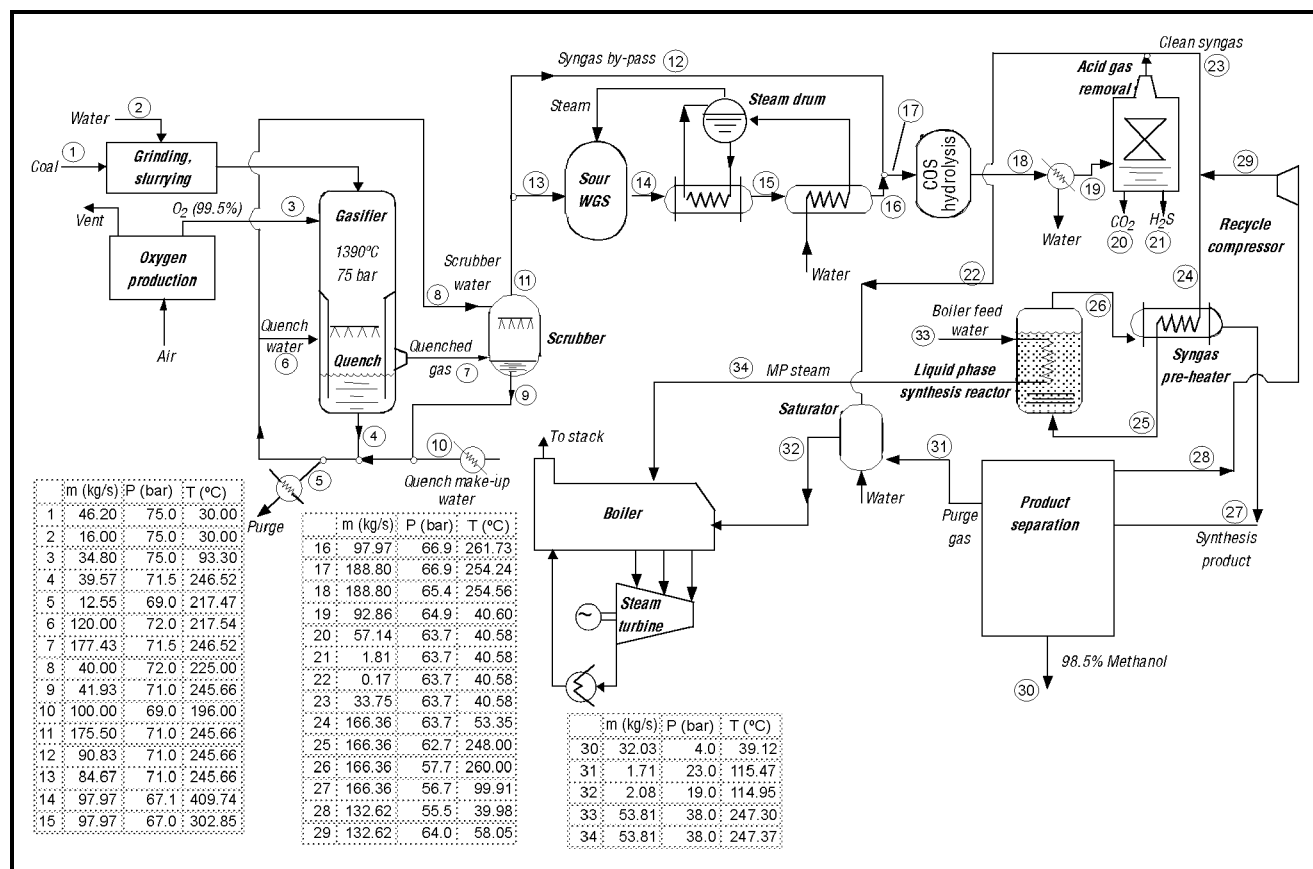


Figure 3. Methanol from coal using liquid-phase synthesis with recycling of unconverted syngas

be defined as the output of methanol divided by a coal input value that is equal to the actual coal input less the amount of coal that would be required to generate the same amount of exportable electricity at a stand-alone electric power plant. The results of this calculation (shown in Table 5) assume an efficiency for stand-alone electric power generation of 43 %, as estimated for a coal integrated gasification/combined cycle (IGCC) plant [Chiesa et al., 2003], for which the electricity production would involve the same (or slightly higher) emissions of air pollutants per kWh as for electricity generated in the OT configuration considered here. The effective efficiencies for the OT cases are lower than the RC efficiencies because the conversion of synthesis gas to liquids is more efficient than conversion to electricity.

### 5.2. Dimethyl ether production

Figure 4 and Table 6 (upper section) give detailed material balances for the once-through DME synthesis plant configuration. Figure 5 and Table 6 (lower section) give balances for the recycle design. These two DME process configurations are similar to the corresponding methanol designs, and the process flow descriptions given above for methanol apply in most respects to the DME designs. One key difference is in the  $H_2:CO$  ratio of the fresh feed gas to the synthesis reactor. In these cases, this ratio is one. Another difference is in the product separation area, where methanol (a by-product of the synthesis reactions) is recovered for recycling back to the synthesis reactor. One additional difference in the product separation area, not shown explicitly in the process diagrams, is the use

of distillation steps (in addition to flash separations). DME separation is considerably more involved than methanol separation because of the greater similarity in physical properties of DME and other gases in the synthesis product stream (especially  $CO_2$ ). The DME product separation area has been modeled on an Air Products design [Air Products, 1993].

Table 7 summarizes the performance estimates for all of the DME cases, each of which has the same coal input rate as for the methanol designs discussed in Section 5.1.3. Comparing the fraction of the coal input energy converted to liquid fuel in the DME OT case (0.25) to that in the methanol OT case (0.23) highlights the synergistic synthesis chemistry of single-step DME production discussed in Section 3.1. Correspondingly, less exportable electricity is generated with DME production. Because of the synergistic synthesis chemistry, the overall efficiency of converting coal to DME plus electricity in the OT case (48 %) is higher than for converting coal to MeOH plus electricity (46 %). In contrast, the efficiency of DME production in the RC case (55 %) is lower than for methanol production (58 %). This is due to the significantly higher on-site electricity requirements for the synthesis and product separation areas with DME production than with MeOH.

## 6. Cost estimates

The above mass and energy balances provided the basis for estimating capital, coal, and non-fuel operating and maintenance costs for each process configuration. Capital

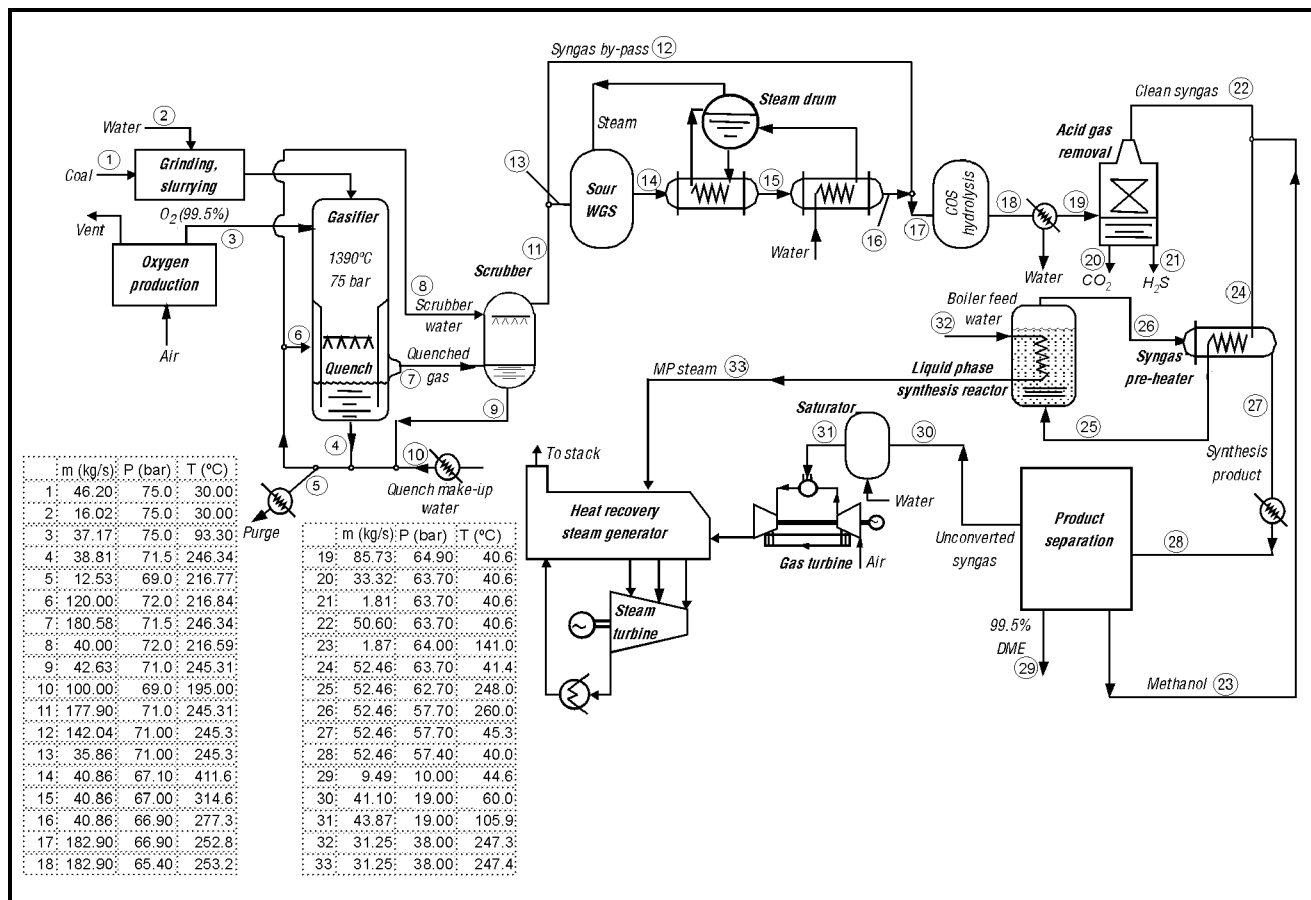


Figure 4. DME and electricity from coal based on "once-through" liquid-phase synthesis

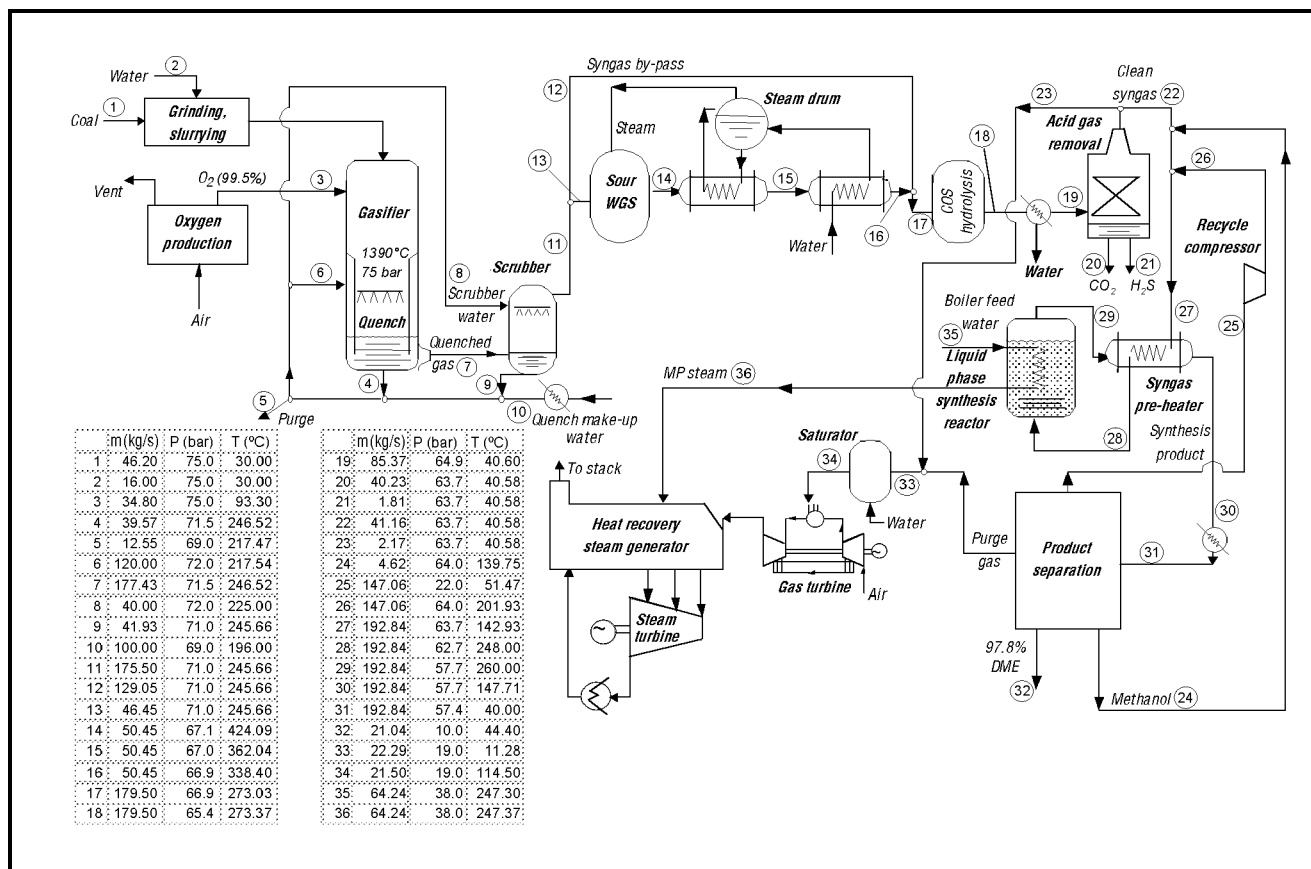


Figure 5. DME from coal using liquid-phase synthesis with recycling of unconverted syngas

Table 6. Material balances for once-through and recycle DME-from-coal processes

	Quench vessel, exit	Water gas shift reactor, inlet	Water gas shift reactor, exit	H <sub>2</sub> S removal unit, inlet	H <sub>2</sub> S removal unit, exit	Total feed into synthesis (inc. recy.)	Recycle gas feed into synthesis	Raw synthesis product	Final liquid product	Fuel gas to gas turbine
<b>Dimethyl ether: once-through synthesis</b>										
Figure 4 stream no.	11	13	14	19	22	25		26	28	30
kg/s	177.90	35.86	40.86	85.73	50.60	52.46	-	52.46	9.49	43.87
kmol/s	9.170	1.848	2.126	4.053	3.149	3.207	-	2.337	0.206	2.226
mol fraction										
CO	0.2021	0.2021	0.0110	0.3709	0.4774	0.4687	-	0.3745	0.0000	0.3931
H <sub>2</sub>	0.1258	0.1258	0.2741	0.3709	0.4774	0.4688	-	0.3534	0.0000	0.3710
CO <sub>2</sub>	0.0430	0.0430	0.2021	0.1845	0.0178	0.0175	-	0.1066	0.0000	0.1119
H <sub>2</sub> O	0.6143	0.6143	0.4999	0.0401	0.0010	0.0010	-	0.0118	0.0000	0.0815
O <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-	0.0000	0.0000	0.0000
N <sub>2</sub>	0.0033	0.0033	0.0028	0.0074	0.0095	0.0093	-	0.0128	0.0000	0.0134
Ar	0.0057	0.0057	0.0049	0.0128	0.0165	0.0162	-	0.0222	0.0000	0.0233
CH <sub>4</sub>	0.0001	0.0001	0.0001	0.0002	0.0003	0.0003	-	0.0004	0.0000	0.0004
H <sub>2</sub> S	0.0054	0.0054	0.0047	0.0131	0.0000	-	-	-	-	-
COS	0.0004	0.0004	0.0003	0.0000	0.0000	-	-	-	-	-
CH <sub>3</sub> OH	-	-	-	-	-	0.0182	-	0.0253	0.0047	4.44E-08
CH <sub>3</sub> OCH <sub>3</sub>	-	-	-	-	-	0.0000	-	0.0929	0.9946	0.0053
<b>Dimethyl ether: recycle synthesis</b>										
Figure 5 stream no.	11	13	14	19	22+23	28	26	29	31	33
kg/s	175.50	46.45	50.45	85.37	43.33	192.84	147.06	192.84	21.04	21.50
kmol/s	9.108	2.411	2.633	4.105	3.042	10.007	6.973	8.156	0.457	0.691
mol fraction										
CO	0.2039	0.2039	0.0143	0.3418	0.4612	0.3981	0.3802	0.3325	0.0000	0.1897
H <sub>2</sub>	0.1271	0.1271	0.2888	0.3925	0.5297	0.3996	0.3539	0.3058	0.0000	0.1556
CO <sub>2</sub>	0.0429	0.0429	0.2117	0.2066	0.0003	0.0866	0.1241	0.1487	0.0000	0.5030
H <sub>2</sub> O	0.6178	0.6178	0.4776	0.0405	0.0011	0.0003	0.0000	0.0146	0.0000	0.1094
O <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N <sub>2</sub>	0.0020	0.0020	0.0018	0.0044	0.0060	0.0811	0.1140	0.0996	0.0000	0.0264
Ar	0.0004	0.0004	0.0004	0.0009	0.0013	0.0148	0.0207	0.0181	0.0000	0.0055
CH <sub>4</sub>	0.0001	0.0001	0.0001	0.0002	0.0003	0.0020	0.0027	0.0024	0.0000	0.0014
H <sub>2</sub> S	0.0054	0.0054	0.0050	0.0129	0.0000	-	-	-	-	-
COS	0.0004	0.0004	0.0004	0.0000	0.0000	-	-	-	-	-
CH <sub>3</sub> OH	-	-	-	-	-	0.0143	0.0176	0.0000	0.0000	0.0000
CH <sub>3</sub> OCH <sub>3</sub>	-	-	-	-	-	0.0031	-	0.0605	0.9997	0.0087

costs ( $\pm 30\%$  accuracy, expressed in 2002 US\$) were estimated for commercially-mature ("Nth plant") systems by major equipment area for manufacture and construction at a United States location primarily based on reference overnight installed costs from one of two sources [Moore, 2003; Kreutz et al., 2003] (Table 8).

The reference capital costs were scaled (using scaling exponents in Table 8) to the capacities corresponding to the plants described in Tables 5 and 7 for methanol and DME, respectively. Since fuel production is of primary interest in the present analysis, to facilitate cost comparisons among different process configurations, we further developed our capital cost estimates for process configurations

producing the same amount of liquid fuel in all cases. We used the fuel output of the recycle case as the common output level. The plant capacities in Tables 5 and 7 for the OT cases have been scaled up accordingly. The resulting plant sizes and installed capital cost estimates are shown in Tables 9 and 10 for methanol and DME respectively. Note 1 in these tables provides some additional details on our cost estimating methodology.

The above capital costs for methanol and DME would be lower if estimated on the basis of Chinese manufacture and construction, rather than on US conditions. For components of ICL processes that in the near future could be manufactured in China (essentially all components except

Table 7. Dimethyl ether summary mass and energy balances with same coal input for all cases

Management of captured CO <sub>2</sub>	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
<b>Coal feed rate</b>						
As-received t/d	3992	3992	3992	3992	3992	3992
Dry t/d	3708	3708	3708	3708	3708	3708
MAF t/d	2958	2958	2958	2958	2958	2958
MW HHV	1134	1134	1134	1134	1134	1134
MW LHV	1085	1085	1085	1085	1085	1085
Carbon in coal, kgC/GJ LHV	25.2	25.2	25.2	25.2	25.2	25.2
<b>Oxygen feed rate</b>						
Total oxidant, t/d	3214	3214	3214	3007	3007	3007
Oxidant purity (mol % O <sub>2</sub> )	94.3	94.3	94.3	99.5	99.5	99.5
Pure O <sub>2</sub> , t/d	3032	3032	3032	2992	2992	2992
<b>Carbon dioxide</b>						
Removed from gas, tCO <sub>2</sub> /d	2631	2631	2631	3221	3221	3221
Captured for storage, tCO <sub>2</sub> /d	0	2276	2631	0	2868	3221
<b>Dimethyl ether product</b>						
Total product output, t/d	820	820	820	1818	1818	1818
Product purity (mol % DME)	99.46	99.46	99.46	99.97	99.97	99.97
MW HHV	268.4	268.4	268.4	658.5	658.5	658.5
MW LHV	269.6	269.6	269.6	599.5	599.5	599.5
MW output relative to recycle case (scale factor)	2.22	2.22	2.22	1.00	1.00	1.00
<b>Electricity</b>						
<b>Gross production (MW)</b>						
Gas turbine	171.8	171.8	171.8	26.5	26.5	26.5
Steam turbine	131.6	131.6	131.6	68.9	68.9	68.9
Syngas expander	3.2	3.2	3.2	11.5	11.5	11.5
Total gross production	306.6	306.6	306.6	106.9	106.9	106.9
<b>On-site consumption (MW)</b>						
Air separation unit <sup>[1]</sup>	50.20	50.20	50.20	48.90	48.90	48.90
Recycle compressor	0	0.00	0.00	32.4	32.40	32.40
Synthesis island	6.20	6.20	6.20	24.60	24.60	24.60
Product separation (included in synthesis)	-	-	-	-	-	-
CO <sub>2</sub> drying/compression <sup>[2]</sup>	0	9.27	11.32	0	11.68	13.72
Balance of plant	2.00	2.00	2.00	2.00	2.00	2.00
Total on-site consumption	58.40	67.67	69.72	107.90	119.58	121.62
<b>Total net sales to grid (MW)</b>	248.2	238.9	236.9	-1.0	-12.7	-14.7
<b>Fraction of coal LHV converted to</b>						
Dimethyl ether	0.248	0.248	0.248	0.552	0.552	0.552
Exportable electricity	0.229	0.220	0.218	-0.001	-0.012	-0.014
Dimethyl ether + electricity	0.477	0.469	0.467	0.551	0.541	0.539
<b>Carbon flows (at 85 % capacity factor)</b>						
Input coal, ktC/yr <sup>[3]</sup>	732	732	732	732	732	732
Captured/stored, ktC/yr	0	193	223	0	243	273
In DME product, ktC/yr	132	132	132	294	294	294
Emissions at plant, kt/yr	600	407	377	438	196	166
<b>Effective dimethyl ether efficiency (LHV)<sup>[4]</sup></b>	53.1	51.0	50.5	55.1	53.8	53.5

1. Air separation was not modeled explicitly. Electricity consumption of 390 kWh/t oxidant was assumed for 99.5 % purity oxidant and 375 kWh/t for 94.3 % purity oxidant.

2. CO<sub>2</sub> drying and compression was not modeled explicitly. Electricity consumption of 97.8 kWh/tCO<sub>2</sub> (or 97.8 kWh/(CO<sub>2</sub>+H<sub>2</sub>S)) was assumed [Chiesa et al., 2003].

3. This is carbon carried into the plant with the coal. Upstream carbon emissions (associated with coal-mining and delivery to the plant) are not included in this number. Upstream emissions are estimated to be 1 kgC/GJ of delivered coal (LHV basis) [Ogden et al., 2004], or 29 ktC/yr (85 % capacity factor) for the plants in this table.

4. The effective efficiency is defined as  $F/(C-E/N)$ , where F is the output of fuel DME (LHV MW), C is the total coal input (LHV MW), E is the exportable electricity production (MW), and N is the efficiency of electricity production from coal (LHV basis) in a stand-alone power plant. In this calculation, the stand-alone power plant is assumed to be an IGCC plant for which N is 43 % [Chiesa et al., 2003].

**Table 8. Reference capital cost estimates by major plant area for commercially-mature (“Nth plant”) technology. (These costs are the basis for the cost estimates in Tables 9 and 10, as described in the captions of those tables<sup>1</sup>.)**

Reference installed overnight cost	(million 2002 \$)	Reference capacity	Scaling exponent
<b>Fuel production area</b>			
Coal-handling and feed	29.10	2367 raw t/d coal	0.67
Gasifier island (dual train)	123.80	1432 MW HHV coal	0.67
Air separation unit <sup>[2]</sup>	64.35	4264 t/d O <sub>2</sub>	0.50
Sour WGS and COS hydrolysis <sup>[3]</sup>	39.30	1450 MW HHV coal	0.67
Sulfur and CO <sub>2</sub> capture (Selexol-based system) <sup>[4]</sup>			
H <sub>2</sub> S removal and stripping, if converted to elemental S	44.44	81 t/d S removed	0.67
H <sub>2</sub> S removal, if co-disposing with CO <sub>2</sub>	24.88	81 t/d S removed	0.67
CO <sub>2</sub> absorption and stripping	43.38	327 t/hr CO <sub>2</sub> removed	0.67
Sulfur recovery (Claus, SCOT plants)	22.90	81 t/d S removed	0.67
CO <sub>2</sub> drying and compression	21.34	292.30 t/hr CO <sub>2</sub> removed	0.67
CO <sub>2</sub> + H <sub>2</sub> S co-drying/co-compression	21.34	292.30 t/hr (CO <sub>2</sub> +H <sub>2</sub> S) removed	0.67
Fuel synthesis and product separation area <sup>[5]</sup>			
Once-through liquid phase MeOH synthesis	20.4	2.89 kmol/s syngas feed to synthesis	0.65
Recycle LP MeOH synthesis	81.77	10.81 kmol/s syngas feed to synthesis	0.65
Methanol product separation/purification	1.72	4.66 kg/s methanol produced	0.291
Once-through liquid phase DME synthesis + purification	36.79	2.91 kmol/s syngas feed to synthesis	0.65
Recycle LP DME synthesis + purification	87.37	8.68 kmol/s syngas feed to synthesis	0.65
Balance of plant for gas production/fuel synthesis area <sup>[2]</sup>	15 % of other fuel area costs		
<b>Power generation area</b>			
Gas turbine generator	58.83	209 gross gas turbine MW <sub>e</sub>	0.67
Heat recovery steam generator + steam turbine-generator	94.70	200 gross steam turbine MW <sub>e</sub>	0.67
Syngas expander	3.10	10 gross expander MW <sub>e</sub>	0.67
Power island balance of plant	57.60	450 gross total MW <sub>e</sub>	0.67

#### Notes

- Unless noted otherwise, the values in this table are taken directly from Kreutz et al. [2003] and account for equipment, installation, general facilities, engineering, overheads, and contingencies.
- Values provided by Moore [2003].
- Kreutz et al. [2003] give a cost estimate for a shift reactor island designed for a plant making pure H<sub>2</sub> from coal. That WGS reactor design includes a high-temperature (adiabatic) stage and a low-temperature (isothermal) stage to maximize CO conversion to H<sub>2</sub>. Our designs utilize only a single high-temperature reactor, since only partial shifting of the CO is required. The high-temperature section of a two-stage WGS system typically accounts for 40 % of the total cost [Moore, 2003]. We have adjusted the original Kreutz-et-al. [2003] WGS cost to account for this.
- Kreutz et al. [2003] report two components of the cost for a Selexol system that removes H<sub>2</sub>S down to levels typically required for IGCC applications (20-50 ppmv) and also removes CO<sub>2</sub>. One part of the cost (H<sub>2</sub>S absorption and stripping) scales with the amount of sulfur absorbed and one part (for CO<sub>2</sub> absorption and stripping) scales with the amount of CO<sub>2</sub> absorbed. If co-disposal of CO<sub>2</sub> and H<sub>2</sub>S is envisioned, the effective cost for the H<sub>2</sub>S section is reduced by 44 %. The cost in this table has been adjusted from the Kreutz-et-al. cost to reflect the lower allowable H<sub>2</sub>S concentration input to a methanol or DME synthesis reactor compared to allowable limits for an IGCC application. It is possible to achieve H<sub>2</sub>S concentrations as low as 1 ppmv with Selexol [Sharp et al., 2002] at a capital cost premium of 10-15 % above the cost of reaching 20-50 ppm [Sharp, 2003]. Augmenting such a system with a sulfur guard bed, at an additional 10-15 % capital cost, enables reaching the ppbv levels of sulfur required for a synthesis feed gas [Sharp, 2003]. Kreutz et al. [2003] sulfur removal costs have been multiplied by 1.15×1.15 to reflect the added cost of reaching more stringent H<sub>2</sub>S concentrations.
- Costs based on scaled-up, “Nth-plant” version of the synthesis reactor operating at the Eastman Chemical facility in Kingsport [Moore, 2003].

the gas turbine), as well as for engineering and construction labor, significant cost reductions are likely to be achievable relative to the estimates in Tables 9 and 10. For example, a pre-feasibility study for construction of an 830,000 t/d facility that would make DME from coal in Ningxia Province, China, indicates that installed capital costs based on US Gulf Coast construction should be multiplied by 0.75 to estimate capital costs for China [Lucas, 2002]. A study of IGCC costs indicates a 0.65 China “location” multiplier on total US overnight installed capital costs for a plant built in China instead of in the USA [Stoll and Todd, 1996]. For gasification projects, Shell China typically applies a location factor of 0.60 to European plant costs, on the basis of its own detailed evalu-

ations of local Chinese manufacturing and construction costs [Wang, 2002].

#### 6.1. Methanol

For plants located in the US, levelized factory-gate production costs for methanol are shown in Table 11. The coal input price for this analysis is \$ 1/GJ<sub>LHV</sub> (\$ 23.5/t). The methanol costs include credits for revenue from exported electricity, assuming the sale price of the electricity is equal to the cost for generating electricity from a new IGCC plant (with no CO<sub>2</sub> capture), for which emissions per kWh of local pollutants such as SO<sub>2</sub> and NO<sub>x</sub> would be somewhat higher than emissions from the methanol-electricity co-production facility (see Table 11, Note 5). For a range of electricity prices, Figure 6 shows the

**Table 9. Estimated total overnight installed capital cost (2002 US\$) for alternative commercially-mature (“Nth plant”) methanol plant configurations with the same methanol production rate in all cases<sup>[1]</sup>**

Management of CO <sub>2</sub> removed from syngas	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
<b>Plant capacities<sup>[2]</sup></b>						
Coal input (MW, LHV)	2748	2748	2748	1085	1085	1085
Methanol output (MW, LHV)	626	626	626	626	626	626
Electricity export (MW)	625	582	577	5	-12	-14
<b>Fuel production area (million 2002 \$)</b>						
Coal handling and feed	93.53	93.53	93.53	41.30	41.30	41.30
Gasifier island (max. unit capacity is 2000 t/d coal in)	239.72	239.72	239.72	105.86	105.86	105.86
Air separation unit	121.96	121.96	121.96	53.90	53.90	53.90
Sour WGS and COS hydrolysis	18.65	18.65	18.65	8.18	8.18	8.18
Sulfur and CO <sub>2</sub> capture (Selexol-based system)						
H <sub>2</sub> S removal and stripping, if converted to elemental S	150.32	150.32	-	66.38	66.38	-
H <sub>2</sub> S removal, if co-disposed with CO <sub>2</sub>	-	-	84.18	-	-	37.17
CO <sub>2</sub> absorption and stripping	64.14	64.14	67.74	28.90	28.90	30.48
Sulfur recovery (Claus, SCOT plants)	77.47	77.47	-	34.21	34.21	0.00
CO <sub>2</sub> drying and compression	-	29.03	-	-	16.18	-
CO <sub>2</sub> + H <sub>2</sub> S co-drying/co-compression	-	-	29.66	-	-	16.52
<b>Fuel synthesis and product separation area</b>						
Once-through liquid phase MeOH synthesis	39.51	39.51	39.51	-	-	-
Recycle LP MeOH synthesis	-	-	-	84.14	84.14	84.14
Methanol product separation/purification	4.21	4.21	4.21	3.01	3.01	3.01
Balance of plant, fuel area	121.43	125.78	104.87	63.88	66.31	57.08
Subtotal for fuel production	930.93	964.32	804.04	489.76	508.37	437.64
<b>Power generation area (million 2002 \$)</b>						
Gas turbine generator	118.20	118.20	118.20	-	-	-
Heat recovery steam generator + steam turbine generator	156.69	156.69	156.69	43.72	43.72	43.72
Syngas expander	-	-	-	-	-	-
Power island balance of plant	99.34	99.34	99.34	15.45	15.45	15.45
Subtotal for power island	374.24	374.24	374.24	59.17	59.17	59.17
<b>Total overnight installed capital cost (million 2002 \$)</b>	<b>1305.16</b>	<b>1338.55</b>	<b>1178.27</b>	<b>548.93</b>	<b>567.53</b>	<b>496.81</b>

**Notes**

1. The cost for each indicated major plant area was estimated beginning with  $COST = COST_{ref} \times (CAPACITY / CAPACITY_{ref})^{SE}$  where the subscript “ref” indicates reference values and exponent “SE” represents scaling exponent, as given in Table 8. CAPACITY (no subscript) refers to the capacity for the particular plant area as calculated from process simulations in which the coal input was fixed at 1085 MW LHV (Table 5). To estimate the cost for plants with larger coal input rates (i.e., for all of the “once-through” plant designs in this table), the values of COST calculated from the above equation were scaled to the larger capacities assuming a scaling exponent of 0.88, except for the fuel synthesis and purification areas and CO<sub>2</sub> (or CO<sub>2</sub>+H<sub>2</sub>S) drying/compression, for which the scaling exponent of 0.65 was used. Moore [2003] recommends a scaling exponent between 0.85 and 0.90 for all but the fuel synthesis/purification areas, since multiple trains of gasifiers, air separation units, etc., would be required at these capacities. For the fuel synthesis/purification area (as well as CO<sub>2</sub> drying/compression), a single train could be used even at the larger sizes, so the scaling exponent of 0.65 was used.
2. Scaled from capacities shown in Table 5 by the ratio of recycle output to once-through outputs shown in that table. The ratio is labeled “scale factor” in Table 5.

methanol cost.

Without considering carbon capture, the least costly methanol (\$ 8.6/GJ) is produced in the RC case. To produce methanol at this cost in the OT case requires an electricity sale price of \$ 0.045/kWh, which is slightly higher than the baseline value used in Table 11 (Figure 6). The cost of methanol is insensitive to electricity price in the RC case (since almost no exportable electricity is produced).

When CO<sub>2</sub> is captured at the plant and injected below ground 100 km from the plant for long-term storage, the

cost of methanol increases relative to the lowest-cost case with CO<sub>2</sub> vented. At the reference electricity sale price, the costs of methanol in the OT and RC cases with CO<sub>2</sub> capture and storage are \$ 11.3/GJ and \$ 9.4/GJ, respectively. When CO<sub>2</sub> and H<sub>2</sub>S are co-captured and stored jointly below ground, the cost of methanol is considerably lower than when CO<sub>2</sub> alone is captured and stored. In fact, the methanol cost is only slightly higher than the cost for the same plant configurations with CO<sub>2</sub> vented. This surprising result is due primarily to the considerably simplified sulfur capture system (including elimination of

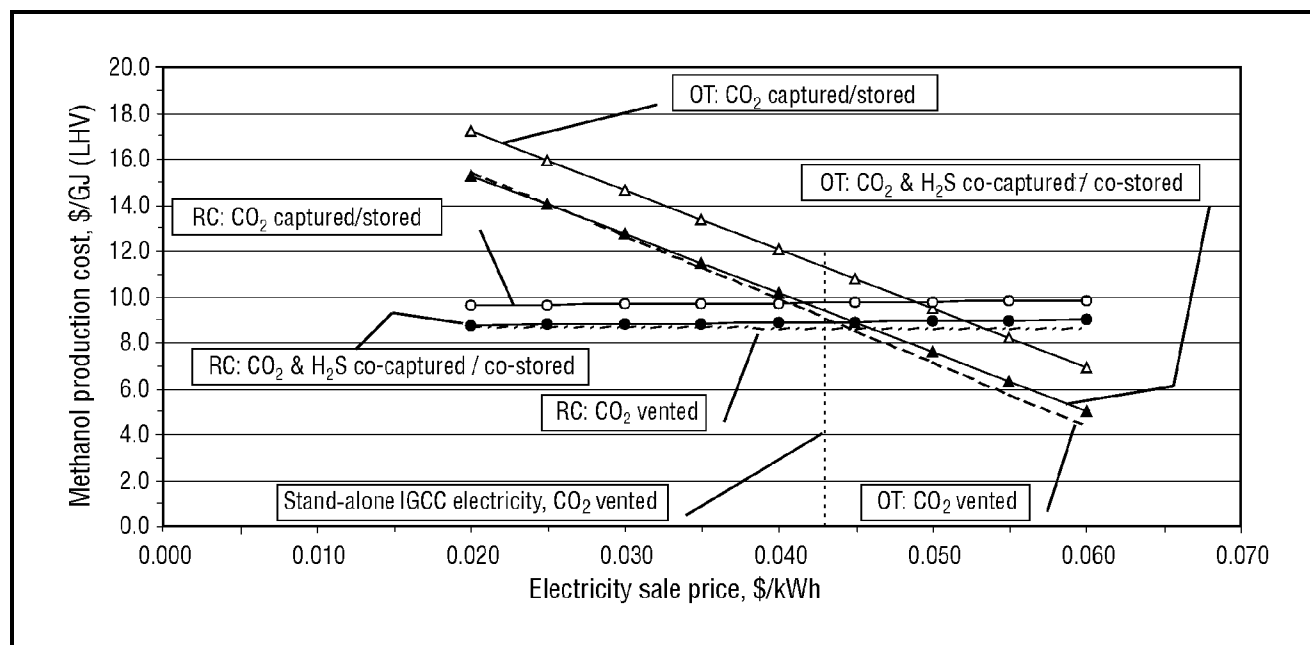


Figure 6. Methanol production costs for alternative plant configurations

the Claus and SCOT units) when  $H_2S$  and  $CO_2$  are co-captured for underground storage.

The methanol costs shown in Table 11 can be compared to the value of methanol as an octane-enhancing gasoline additive and to the cost of methanol as a neat fuel (100 % methanol) used in vehicles replacing petroleum-gasoline vehicles.

When used as a gasoline additive, methanol will boost fuel octane without significantly affecting engine efficiency. Thus, the value of methanol as an additive can be estimated from the difference in value between a regular-grade gasoline and a mid-grade gasoline. Consider the case of Beijing on April 11, 2003 (when the world crude oil price was about \$ 23/bbl = \$ 169/t; 1 bbl or barrel = about 136 kg). The average refinery-gate price (including taxes) for regular-grade gasoline (90 octane) from 36 large refineries in China on that date was 3172 RMB/t (or \$ 0.287/l) [Changchun, 2003]. The mid-grade (93 octane) gasoline wholesale price that same day was 3408 RMB/t (\$ 0.308/l). Since methanol has a blending octane of 120 [Wyman et al., 1993], a 10 % volume addition of methanol to 90-octane gasoline would increase the octane of the blended fuel to 93, and the added methanol would have a value of \$ 0.50/l, or \$ 28/GJ<sub>LHV</sub><sup>[5]</sup>. While the value of methanol in this application would be far above the estimated production cost, the market potential of this application is limited by fuel blending limits.

Much larger potential markets are for methanol as a neat fuel or as M85 (85 % MeOH, 15 % gasoline). The value of methanol in a neat application will depend on the efficiency of the methanol engine relative to a conventional gasoline engine. An optimized spark-ignited neat-methanol engine will be more energy-efficient than a conventional gasoline spark-ignited engine primarily because of higher compression ratios that can be achieved with methanol. Wyman et al. [1993] indicate that a 20 % engine efficiency advantage can be expected. Conserva-

tively, we consider a 15 % gain here, which gives methanol production costs of \$ 0.24–0.25/l gasoline-equivalent for the cases with  $CO_2$  venting and \$ 0.25–0.32/l gasoline-equivalent for process configurations with  $CO_2$  capture (Table 11). These values can be compared with average Chinese refinery-gate gasoline prices mentioned above (\$ 0.29–0.31/l). As another comparison, the average sale price of petroleum gasoline by US refiners to resellers<sup>[6]</sup> in April 2003 was \$ 0.26/l [EIA, 2003]. These comparisons suggest that the methanol costs shown in Table 11 (even for some cases with  $CO_2$  capture and storage) would be competitive with gasoline made from crude oil when the world oil price is \$ 23/bbl or more, particularly considering that capital costs for methanol plants built in China would be lower than those estimated in this analysis (for reasons discussed at the start of Section 6).

### 6.2. Dimethyl ether

For plants located in the US, levelized factory-gate production costs for DME are shown in Table 12 for the same input parameter values as discussed above for methanol, including electricity sold for \$ 0.429/kWh. For other electricity prices, Figure 7 shows DME costs as a function of electricity sale price.

Without considering carbon capture cases, DME produced in the OT case (\$ 8.7/GJ) is less costly than in the RC case (\$ 9.5/GJ). The “break-even” electricity price for the once-through versus recycle configurations is \$ 0.040/kWh, which is below the assumed reference electricity sale price.

When  $CO_2$  is captured and stored, the calculated costs of DME in the OT and RC cases are \$ 10.0/GJ and \$ 10.4/GJ, respectively, using the reference electricity price. When  $CO_2$  and  $H_2S$  are co-captured/co-stored, the DME cost in the OT case is 21 % lower than with capture of  $CO_2$  alone, and the DME cost in the RC case is 8 % lower than with  $CO_2$  capture alone.

Moreover, in the RC case with co-capture/co-storage,

**Table 10. Estimated total overnight installed capital cost (2002 US\$) for alternative commercially-mature (“Nth plant”) DME plant configurations with same the DME production rate in all cases<sup>[1]</sup>**

Management of CO <sub>2</sub> removed from syngas	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
<b>Plant capacities<sup>[2]</sup></b>						
Coal input (MW, LHV)	2414	2414	2414	1085	1085	1085
DME output (MW, LHV)	600	600	600	600	600	600
Electricity export (MW)	552	531	527	-1	-13	-15
<b>Fuel production area (million 2002 \$)</b>						
Coal-handling and feed	83.44	83.44	83.44	41.30	41.30	41.30
Gasifier island (dual train)	213.86	213.86	213.86	105.86	105.86	105.86
Air separation unit	109.63	109.63	109.63	53.90	53.90	53.90
Sour WGS and COS hydrolysis	9.21	9.21	9.21	5.47	5.47	5.47
Sulfur and CO <sub>2</sub> capture (Selexol-based system)						
H <sub>2</sub> S removal and stripping	134.12	134.12	-	66.38	66.38	-
H <sub>2</sub> S removal, co-disposal with CO <sub>2</sub>	-	-	75.11	-	-	37.17
CO <sub>2</sub> absorption and stripping	38.22	38.22	42.11	22.08	22.08	23.87
Sulfur recovery (Claus, SCOT plants)	69.12	69.12	-	34.21	34.21	-
CO <sub>2</sub> drying and compression	-	18.59	-	-	12.67	-
CO <sub>2</sub> + H <sub>2</sub> S co-drying/co-compression	-	-	19.28	-	-	13.05
<b>Fuel synthesis and product separation area</b>						
Once-through liquid phase DME synthesis + purification	65.88	65.88	65.88	-	-	-
Recycle LP DME synthesis + purification	-	-	-	95.83	95.83	95.83
Balance of plant, fuel area	108.52	111.31	92.78	63.75	65.65	56.47
Subtotal for fuel production	832.01	853.39	711.31	488.78	503.35	432.93
<b>Power generation area (million 2002 \$)</b>						
Gas turbine generator	104.35	104.35	104.35	15.69	15.69	15.69
Heat recovery steam generator + steam turbine generator	144.54	144.54	144.54	46.37	46.37	46.37
Syngas expander	2.92	2.92	2.92	3.40	3.40	3.40
Power island balance of plant	89.99	89.99	89.99	21.99	21.99	21.99
Subtotal for power island	341.80	341.80	341.80	87.45	87.45	87.45
<b>Total overnight installed capital cost (million 2002 \$)</b>	<b>1173.81</b>	<b>1195.20</b>	<b>1053.11</b>	<b>576.24</b>	<b>590.81</b>	<b>520.38</b>

**Notes**

- The cost for each indicated major plant area was estimated beginning with  $COST = COST_{ref} \times (CAPACITY / CAPACITY_{ref})^{SE}$  where the subscript “ref” indicates reference values and exponent “SE” represents scaling exponent, as given in Table 8. CAPACITY (no subscript) refers to the capacity for the particular plant area as calculated from process simulations in which the coal input was fixed at 1085 MW LHV (Table 7). To estimate the cost for plants with larger coal input rates (i.e., for all of the “once-through” plant designs in this table), the values of COST calculated from the above equation were scaled to the larger capacities assuming a scaling exponent of 0.88, except for the fuel synthesis and purification areas and CO<sub>2</sub> (or CO<sub>2</sub>+H<sub>2</sub>S) drying/compression, for which the scaling exponent of 0.65 was used. Moore [2003] recommends a scaling exponent between 0.85 and 0.90 for all but the fuel synthesis/purification areas, since multiple trains of gasifiers, air separation units, etc., would be required at these capacities. For the fuel synthesis/purification area (as well as CO<sub>2</sub> drying/compression), a single train could be used even at the larger sizes, so the scaling exponent of 0.65 was used.
- Scaled from capacities shown in Table 7 by the ratio of recycle output to once-through outputs shown in that table. The ratio is labeled “scale factor” in Table 7.

there is essentially no cost penalty for carbon capture relative to the RC configuration with CO<sub>2</sub> venting. In the OT case with co-capture/co-storage, there is actually a cost advantage compared to the OT case with CO<sub>2</sub> vented. This is unlike the case for methanol production (Table 11), where the methanol cost in the OT case with CO<sub>2</sub> co-capture/co-storage is higher than for the OT case with CO<sub>2</sub> vented. The advantageous relative costs for DME arise from the fact that less CO<sub>2</sub> is captured and stored in the OT case for DME than for methanol (7.7 kgC/GJ<sub>DME</sub> and 13.1 kgC/GJ<sub>MeOH</sub>).

The above DME costs are also expressed in Table 12

on LPG-equivalent, diesel-equivalent, and gasoline-equivalent bases.

The LPG-equivalent costs, ranging from \$ 399/t to \$ 437/t when CO<sub>2</sub> is vented and from \$ 380/t to \$ 478/t when CO<sub>2</sub> is captured and stored, can be compared with costs of LPG in China. Typical ex-refinery wholesale prices of LPG at Chinese refineries were 2980-3370 RMB/t in April 2003 [Cui, 2003], or an average of US\$ 383/t. Wholesale prices of imported LPG at coastal terminals in China were in this same range. Since the LPG-equivalent DME costs in Table 12 are based on a USA plant location, it is likely that a plant located in China

Table 11. Levelized production costs for methanol with alternative process configurations

Management of CO <sub>2</sub> removed from syngas	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
Methanol output (MW, LHV)	626	626	626	626	626	626
Net electricity output (MW)	625	582	582	5	-12	-14
Coal input (MW)	2748	2748	2748	1085	1085	1085
Total capital required, overnight construction (million \$)	1305	1339	1178	549	568	497
CO <sub>2</sub> transport/storage cost <sup>[1]</sup> , \$/tCO <sub>2</sub>	-	4.93	4.71	-	6.72	6.43
<b>Methanol production cost (\$/GJ, LHV)</b>						
Capital charge <sup>[2]</sup>	13.53	13.88	12.21	5.69	5.88	5.15
Operation and maintenance <sup>[3]</sup>	3.11	3.19	2.81	1.31	1.35	1.18
Coal feedstock <sup>[4]</sup>	4.39	4.39	4.39	1.73	1.73	1.73
Electricity co-product credit <sup>[5]</sup>	-11.91	-11.10	-11.00	-0.10	0.24	0.27
CO <sub>2</sub> disposal	0.00	0.96	0.99	0.00	0.53	0.55
Total production cost (\$/GJ, LHV)	9.12	11.32	9.41	8.64	9.74	8.89
Total, \$/t	181	225	187	172	194	177
Total, \$/gallon	0.62	0.77	0.64	0.59	0.67	0.61
<b>MeOH Cost, gasoline-equivalent basis</b>						
\$/GJ gasoline equivalent <sup>[6]</sup>	7.93	9.85	8.18	7.51	8.47	7.73
\$/gallon gasoline-equivalent	0.96	1.20	0.99	0.91	1.03	0.94
\$/l gasoline-equivalent	0.25	0.32	0.26	0.24	0.27	0.25

Notes

- The CO<sub>2</sub> disposal cost has been estimated as a function of the rate of CO<sub>2</sub> disposal based on Ogden [2002]. CO<sub>2</sub> (available at 150 bar at the plant gate) is piped 100 km and injected 2 km below ground into a saline aquifer. The assumed maximum per-well injection capacity is 2500 t/d of CO<sub>2</sub>.
- Assuming 16 % of the overnight cost as interest during construction (4-year construction, 10 % interest rate), 15 % annual capital charge rate, and 85 % capacity factor.
- Annual non-fuel operating and maintenance cost is assumed to be 4 % of overnight installed capital cost.
- For a coal price of \$ 1/GJ<sub>LHV</sub> (\$ 23.5/t as-received).
- For electricity sale price of \$ 0.0429/kWh, the estimated production cost (using the parameter assumptions given in Notes 2, 3, and 4) of electricity generated by a new IGCC power plant (with CO<sub>2</sub> vented) with capacity 390.1 MW and overnight installed capital cost of \$ 1203/kW [Kreutz et al., 2003].
- Neat methanol engines are assumed to be 15 % more efficient than conventional gasoline spark-ignited engines [Fleisch et al., 1997].

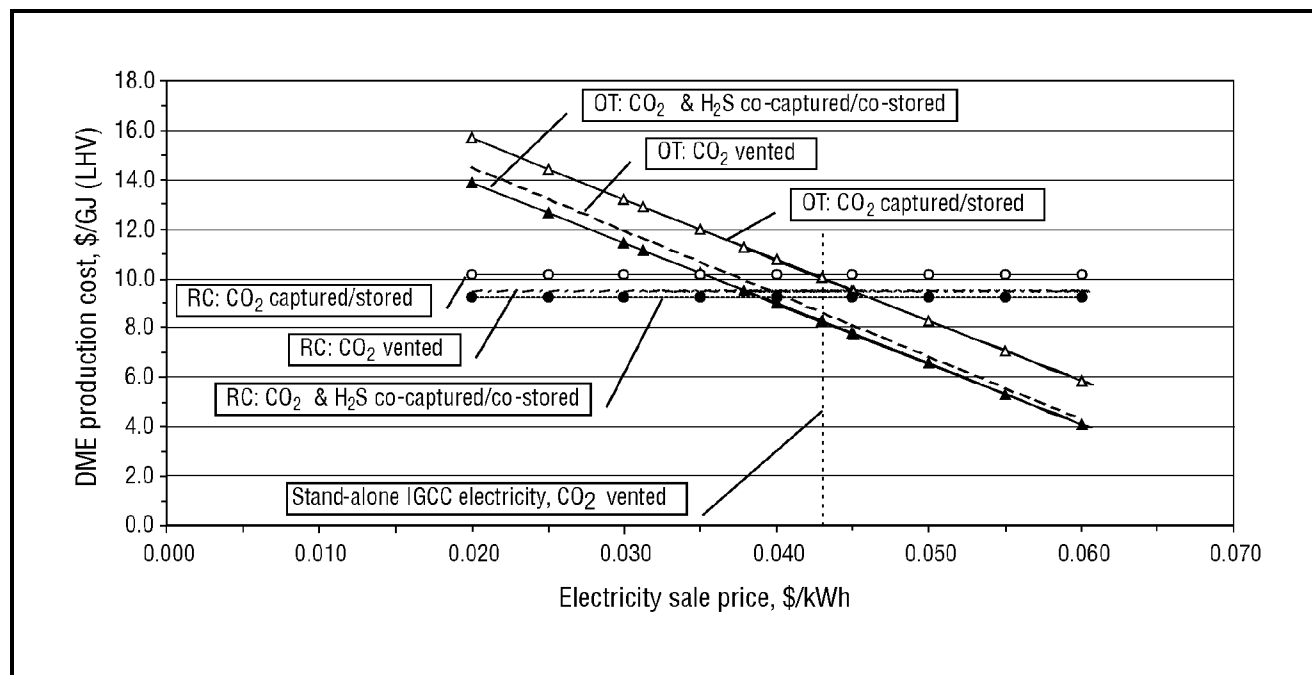


Figure 7. DME production costs for alternative plant configurations

Table 12. Levelized production costs for DME with alternative process configurations

Management of CO <sub>2</sub> removed from syngas	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
DME output (MW, LHV)	600	600	600	600	600	600
Net electricity output (MW)	552	531	527	-1.0	-13	-15
Coal input (MW)	2414	2414	2414	1085	1085	1085
Total capital required, overnight construction (million \$)	1174	1195	1053	576	591	520
CO <sub>2</sub> transport/storage cost <sup>[1]</sup> , \$/tCO <sub>2</sub>	-	6.66	6.13	-	8.45	7.90
<b>DME production cost (\$/GJ, LHV)</b>						
Capital charge <sup>[2]</sup>	12.71	12.94	11.40	6.24	6.40	5.63
Operation and maintenance <sup>[3]</sup>	2.92	2.97	2.62	1.43	1.47	1.30
Coal feedstock <sup>[4]</sup>	4.03	4.03	4.03	1.81	1.81	1.81
Electricity co-product credit <sup>[5]</sup>	-10.98	-10.57	-10.48	0.02	0.25	0.29
CO <sub>2</sub> disposal	0.00	0.65	0.69	0.00	0.47	0.49
Total production cost (\$/GJ, LHV)	8.68	10.02	8.26	9.50	10.40	9.52
Total, \$/t	247	286	235	271	296	271
<b>DME cost, LPG-equivalent basis, \$/t LPG-equiv.<sup>[6]</sup></b>	399	461	380	437	478	438
<b>DME cost, diesel-equivalent basis</b>						
\$/GJ diesel-equivalent	8.68	10.02	8.26	9.50	10.40	9.52
\$/gallon diesel-equivalent	1.18	1.36	1.12	1.29	1.41	1.29
\$/l diesel-equivalent	0.30	0.35	0.29	0.33	0.36	0.33
<b>DME cost, gasoline-equivalent basis</b>						
\$/GJ gasoline equivalent <sup>[7]</sup>	7.32	8.46	6.97	8.02	8.77	8.04
\$/gallon gasoline-equivalent	0.89	1.03	0.85	0.97	1.07	0.98
\$/l gasoline-equivalent	0.23	0.27	0.22	0.26	0.28	0.26

## Notes

1. The estimated CO<sub>2</sub> disposal cost as a function of the rate of CO<sub>2</sub> disposal is based on Ogden [2002]. CO<sub>2</sub> (available at 150 bar at the plant gate) is piped 100 km and injected 2 km below ground into a saline aquifer. The assumed maximum per-well injection capacity is 2500 t/d of CO<sub>2</sub>.
2. Assuming 16 % of the overnight cost as interest during construction (4-year construction, 10 % interest rate), 15 % annual capital charge rate, and 85 % capacity factor.
3. Annual non-fuel operating and maintenance cost is assumed to be 4 % of overnight installed capital cost.
4. For a coal price of \$ 1/GJ<sub>LHV</sub> (\$ 23.5/t as-received).
5. For electricity sale price of \$ 0.0429/kWh, the estimated production cost (using the parameter assumptions given in Notes 2, 3, and 4) of electricity generated by a new IGCC power plant (with CO<sub>2</sub> vented) with capacity 390.1 MW and overnight installed capital cost of \$ 1203/kW [Kreutz et al., 2003].
6. This takes into consideration the difference in heating value between DME (28.5 MJ/kg, LHV) and LPG (46 MJ/kg, LHV).
7. A DME compression-ignition vehicle is assumed to have an 18.5 % efficiency advantage relative to a conventional gasoline spark-ignited engine vehicle [Weiss et al., 2003].

would produce DME at costs that would be very competitive with wholesale LPG prices.

The above LPG and DME costs can also be compared with estimated health-related costs of indoor air pollution arising from cooking with solid fuels, which the World Health Organization ranks as the eighth most serious contributor to the total burden of disease in “low-mortality developing countries” (which includes China) [WHO, 2002]. The World Bank has estimated that the annual health cost of indoor air pollution in rural China was between \$ 3.7 and \$ 10.6 billion in 1995 [World Bank, 1997]. Cooking with a clean liquid or gas fuel (e.g., LPG or DME) would eliminate most, if not all, of this health cost. Since average annual per-capita cooking fuel requirements with gas or liquid fuels in China are estimated to be between 1.6 GJ/cap/yr [Lucas, 2002] and 3.4 GJ/cap/yr [Lui et al., 2001] (or 34 to 73 kg LPG/cap/yr),

the estimated health damage costs are equivalent to \$ 470 to \$ 2900/t of LPG-equivalent cooking fuel provided to the entire exposed population considered in the World Bank study<sup>[7]</sup>. Thus, the costs of DME production estimated above would appear to be lower – in fact, far lower – than the cost of health damage wrought by the indoor use of solid fuels for cooking in rural China.

As a transportation fuel, DME used in a compression-ignition engine would have an estimated 10 % efficiency advantage relative to a petroleum-diesel engine if low NO<sub>x</sub> emissions are an objective [Fleisch et al., 1997]. The DME cost on a \$/l diesel-equivalent basis in Table 12 neglects the cost impact of this advantage, assuming instead that it would be offset by added infrastructure-related costs for DME delivery to vehicles. (Table 12 also neglects the value of reduced emissions of other tailpipe pollutants with DME relative to diesel fuel, especially

health-damaging small particles.) The lowest diesel-equivalent production cost in Table 12 is \$ 0.29/l. For comparison, the average sale price of petroleum-derived No. 2 diesel fuel charged by US refiners to resellers in April 2003 was \$ 0.23/l [EIA, 2003], so DME as replacement fuel for diesel-engine vehicles does not appear especially cost-competitive when the world crude oil price is \$ 23/bbl or less, at least for the US cost conditions considered here.

However, the high cetane rating of DME may widen the appeal of compression-ignition automobiles [Williams and Larson, 2003]<sup>[8]</sup>, so a comparison of DME as a compression-ignition engine fuel with gasoline for spark-ignition engines may be appropriate. In this case, Weiss et al. [2003] indicate an 18.5 % efficiency advantage for the compression-ignition engine. (Fleisch et al. [1997] indicate a 30-40 % efficiency improvement.) Considering an 18.5 % advantage, the cost of DME on a gasoline-equivalent basis would be \$ 0.23-0.26/l gasoline-equivalent in cases when CO<sub>2</sub> is vented and \$ 0.22-0.28/l gasoline-equivalent when CO<sub>2</sub> is captured and stored (Table 12). As noted earlier, the average sale price of petroleum gasoline by US refiners to resellers in April 2003 was \$ 0.26/l [EIA, 2003], which suggests that with the costs shown in Table 12 (even for some cases with CO<sub>2</sub> capture and storage) DME vehicles could be competitive replacements for gasoline-engine vehicles with only modest world oil prices (\$ 23/bbl or more). The cost advantage for DME would be larger than shown here when a China location factor is taken into consideration (as noted earlier).

## 7. Carbon emissions

An important longer-term consideration for transportation fuels provided by ICL processes is the carbon emissions that would result from a switch from petroleum to coal-based fuels. Because of the high carbon content of coal per unit of energy, fuels produced by ICL will lead to considerably higher carbon emissions to the atmosphere than petroleum-derived fuels if carbon capture and storage are not included as part of the ICL plant design. Conversely, if carbon capture is utilized, then carbon emissions can be lower than with petroleum-derived fuels.

There is no unique means for allocating carbon emissions to different products from a polygeneration plant. In the following analysis, for the OT cases, we have chosen to allocate to the liquid fuel product the carbon embodied in the fuel itself (18.8 kgC/GJ<sub>LHV</sub> for MeOH and 18.3 kgC/GJ<sub>LHV</sub> for DME) plus an appropriate fraction of carbon emissions associated with upstream coal-processing (mining and transportation to the plant). All other emissions are charged to electricity production. For the RC cases we allocate all emissions to the liquid fuel output, since there is little or no export electricity. Table 13 shows the resulting carbon emissions.

The upper portion of Table 13 shows specific carbon emissions (per GJ of fuel and per kWh electricity) both in absolute terms and as percentages of specific emissions

associated with alternative petroleum-based fuels and alternative stand-alone coal-electricity generation technologies. The lower portion of the table shows total carbon emissions as a percentage of total emissions with the alternative of petroleum-based fuels and stand-alone coal power generation for the same total equivalent GJ of fuel and total kWh of electricity as produced by the ICL process. For the RC cases, total emissions as a percentage of petroleum-fuel emissions are identical to the specific emissions as percentage of specific petroleum fuel emissions, since there is no electricity co-product in the RC cases. In the OT cases, the total emissions relative to total emissions for petroleum fuels plus stand-alone electricity generation are the weighted average of the specific emissions, with the total amount of fuels and electricity produced in the ICL process used for the weighting. Table 13 shows the following.

With no CO<sub>2</sub> capture/storage, total carbon emissions are:

- in the MeOH OT case, 106 % to 127 % of emissions for gasoline plus stand-alone electricity (SAE);
- in the MeOH RC case, 154 % of gasoline emissions;
- in the DME OT case, 106-128 % of emissions with diesel plus SAE emissions, or 102-122 % of gasoline plus SAE emissions; and
- in the DME RC case, 181 % of diesel emissions or 156 % of gasoline emissions.

With CO<sub>2</sub> capture/storage separate from H<sub>2</sub>S capture, total carbon emissions are:

- in the MeOH OT case, 60 % to 72 % of emissions for gasoline plus stand-alone electricity (SAE);
- in the MeOH RC case, 81 % of gasoline emissions;
- in the DME OT case, 82-98 % of emissions with diesel plus SAE emissions, or 78-94 % of gasoline plus SAE emissions; and
- in the DME RC case, 124 % of diesel emissions or 107 % of gasoline emissions.

With CO<sub>2</sub>/H<sub>2</sub>S co-capture/co-storage, total carbon emissions are:

- in the MeOH OT case, 56 % to 67 % of emissions for gasoline plus stand-alone electricity (SAE);
- in the MeOH RC case, 75 % of gasoline emissions;
- in the DME OT case, 78-94 % of emissions with diesel plus SAE emissions, or 75-89 % of gasoline plus SAE emissions; and
- in the DME RC case, 116 % of diesel emissions or 100 % of gasoline emissions.

Thus, without CO<sub>2</sub> capture, carbon emissions will be up to 28 % higher for once-through ICL processes than for the alternative of using petroleum fuels and producing electricity at a stand-alone power plant. The carbon penalty is even more severe with recycle ICL processes, for which carbon emissions will be up to 81 % more than when using petroleum fuel.

When some CO<sub>2</sub> is captured in the ICL processes, carbon emissions can likely be reduced below those with the alternative of petroleum fuel and stand-alone electricity. The potential for reduced emissions is considerably greater with once-through ICL processes than with the RC processes.

Table 13. Carbon emissions

	Once-through (OT)			Recycle (RC)		
	Vent	Capture	Co-capture	Vent	Capture	Co-capture
<b>Specific carbon emissions for ICL processes relative to petroleum fuels and stand-alone coal electricity generation</b>						
	<b>Methanol</b>					
<b>Methanol engine replacing petroleum-gasoline engine<sup>[1]</sup></b>						
C emissions charged to MeOH, kgC/GJ <sup>[2]</sup>	20.90	21.06	21.08	45.38	23.76	21.97
C emissions charged to MeOH, kgC/GJ gasoline-equiv.	18.17	18.31	18.33	39.46	20.66	19.11
% of petroleum-gasoline emissions <sup>[3]</sup>	71	72	72	154	81	75
<b>Electricity from OT polygen. replacing IGCC or coal-steam electricity</b>						
Carbon emissions charged to electricity, kgC/kWh	0.339	0.158	0.141	-	-	-
% of coal-steam electric plant emissions <sup>[4]</sup>	119	55	49	-	-	-
% of IGCC electricity emissions <sup>[4]</sup>	154	72	64	-	-	-
	<b>DME</b>					
<b>DME engine replacing petroleum-diesel engine<sup>[5]</sup></b>						
Carbon charged to DME, kgC/GJ <sup>[2]</sup>	20.18	20.26	20.28	47.38	32.27	30.41
Carbon charged to DME, kgC/GJ diesel equivalent	20.18	20.26	20.28	47.38	32.27	30.41
% of petroleum-diesel carbon emissions <sup>[3]</sup>	77	78	78	181	124	116
<b>DME engine replacing petroleum-gasoline engine<sup>[6]</sup></b>						
Carbon charged to DME, kgC/GJ <sup>[2]</sup>	20.18	20.26	20.28	47.38	32.27	30.41
Carbon charged to DME, kgC/GJ gasoline equivalent	17.03	17.10	17.11	39.99	27.24	25.66
% of petroleum-gasoline carbon emissions <sup>[3]</sup>	67	67	67	156	107	100
<b>Electricity from OT polygen. replacing IGCC or coal-steam electricity</b>						
Carbon charged to electricity, kgC/kWh	0.333	0.237	0.222	-	-	-
% of coal-steam electric plant carbon emissions <sup>[4]</sup>	117	83	78	-	-	-
% of IGCC electricity carbon emissions <sup>[4]</sup>	152	108	101	-	-	-
<b>Total carbon emissions for ICL processes relative to equivalent petroleum fuels and stand-alone coal electricity generation<sup>[7]</sup></b>						
	<b>Methanol</b>					
RC MeOH vs. petroleum gasoline	-	-	-	154	81	75
OT MeOH vs. petroleum gasoline + OT electricity vs. coal-steam electricity	106	60	56	-	-	-
OT MeOH vs. petroleum gasoline + OT electricity vs. coal IGCC electricity	127	72	67	-	-	-
	<b>DME</b>					
RC DME vs. petroleum diesel	-	-	-	181	124	116
OT DME vs. petroleum diesel + OT electricity vs. coal-steam electricity	106	82	78	-	-	-
OT DME vs. petroleum diesel + OT electricity vs. coal IGCC electricity	128	98	94	-	-	-
RC DME vs. petroleum gasoline	-	-	-	156	107	100
OT DME vs. petroleum gasoline + OT electricity vs. coal-steam electricity	102	78	75	-	-	-
OT DME vs. petroleum gasoline + OT electricity vs. coal IGCC electricity	122	93	89	-	-	-

**Notes**

1. A methanol engine is assumed to have a 15 % efficiency advantage over a gasoline engine.
2. This is the carbon embodied in the liquid fuel (18.8 kgC/GJ<sub>LHV</sub> for MeOH and 18.3 kgC/GJ<sub>LHV</sub> for DME) plus a fraction of the upstream emissions associated with coal-mining and transportation (1 kgC/GJ<sub>coal,LHV</sub>) [Ogden et al., 2004]. The fraction of upstream emissions allocated to the liquid fuel is  $[1-(N_{OT}/N_{SA})]$ , where  $N_{OT}$  is the electricity generation efficiency of the polygeneration plant and  $N_{SA}$  is the generating efficiency for a stand-alone IGCC plant (43 %).
3. Including all upstream emissions associated with crude oil production and delivery to refinery, refining, fuel delivery to vehicle, and fuel combustion in the vehicle, the carbon emissions for petroleum gasoline (reformulated gasoline with methyl tertiary-butyl ether (MTBE) and meeting 30 ppm sulfur emissions specification) are 25.66 kgC/GJ<sub>LHV</sub> and for petroleum diesel (low-sulfur diesel) they are 26.11 kgC/GJ<sub>LHV</sub> [Wang, 2003].
4. With the same coal as used with the polygeneration plants, the carbon emissions for a 43 % efficient IGCC (including upstream emissions associated with coal-mining and delivery) are 0.219 kgC/kWh. For a coal-steam electric plant (33 % efficiency), the emissions are 0.286 kgC/kWh.
5. A DME engine is assumed to have the same efficiency as a petroleum-diesel engine.
6. A DME engine is assumed to have a 18.5 % efficiency advantage relative to a petroleum-gasoline engine, which is the estimated efficiency advantage of an advanced diesel engine relative to an advanced gasoline engine [Weiss et al., 2003].
7. For the RC cases, the relative total emissions are the same as the relative specific emissions. For the OT cases, the relative total emissions are the average of relative emissions for fuels and of relative emissions for electricity, weighted by the total amounts of fuels and electricity produced.

## 8. Summary

Technology for indirect coal liquefaction using oxygen-blown gasification and liquid-phase synthesis is commercially ready, with several commercial projects in the planning stages worldwide. The energy conversion efficiency of ICL process designs described in detail in this paper are 58 % for methanol (lower heating value basis) and 55 % for dimethyl ether when the only product of the facility is a liquid fuel. In these designs, synthesis gas that is unconverted after passing through the synthesis reactor is recycled back to the reactor to increase conversion. A water gas shift reactor is used upstream of the synthesis reactor to increase the H<sub>2</sub>/CO ratio of the syngas to optimize the CO conversion rate in the synthesis reactor. In ICL configurations using “once-through” synthesis, co-product electricity is generated from the unconverted synthesis gas after a single pass through the reactor. Electricity is a major co-product in these designs.

Because in all designs some CO<sub>2</sub> must be removed (together with all H<sub>2</sub>S) from the syngas before the synthesis reactor, a relatively pure stream of CO<sub>2</sub> is available at these ICL facilities. This CO<sub>2</sub> could be vented to the atmosphere. Alternatively, it could be captured (alone or together with the H<sub>2</sub>S) and compressed to a suitable pressure (150 bar) for pipeline transport to an underground storage site. A small efficiency penalty would be paid for this capture and compression. For example, the efficiencies noted in the previous paragraph for recycle ICL configurations would be reduced by about two percentage points.

With capital cost estimates based on manufacturing, construction, and operation of the ICL facilities in the United States, the estimated cost of methanol production (recycle configuration, with CO<sub>2</sub> vented) is \$ 8.6/GJ<sub>LHV</sub> (\$ 0.16/l or \$ 172/t). Considering methanol as an automotive fuel, for which the engine efficiency advantage over a conventional gasoline engine is an estimated 15 %, this production cost is equivalent to \$ 0.24/l gasoline-equivalent. For comparison, \$ 0.24/l was the refiner wholesale price of motor gasoline in the United States in April 2003 (when the world crude oil price was about \$ 23/bbl.)

For “once-through” process configurations, the methanol production cost depends on the revenue generated by sale of the co-product electricity. For the once-through configurations in this analysis with venting of CO<sub>2</sub>, the cost of methanol is less than the cost at a recycle-based facility when the electricity sale price is less than \$ 0.045/kWh. The co-produced electricity would have no sulfur or particulate emissions associated with it, and from this perspective should be of higher value than electricity generated by an IGCC system, the cleanest commercially-available coal-electric technology. The estimated cost for IGCC electricity (using cost assumptions consistent with those used for the ICL analysis) is \$ 0.043/kWh.

When CO<sub>2</sub> is captured for underground storage, the cost of methanol increases (compared to the least costly case with CO<sub>2</sub> venting) by 3-13 % in the recycle cases and by 8-31 % in the once-through cases (with co-product elec-

tricity sold for \$ 0.043/kWh).

For DME production based on US conditions, the least costly DME (when CO<sub>2</sub> is vented) is produced in a once-through design (\$ 8.7/GJ<sub>LHV</sub> or \$ 250/t). For the recycle case, the cost is \$ 9.5/GJ<sub>LHV</sub> (\$ 271/t). DME is less costly with a once-through configuration than with a recycle configuration as long as the electricity sale price is below \$ 0.04/kWh. When CO<sub>2</sub> is captured and stored, the calculated costs of DME increase by 10-20 % with the recycle designs compared to the least costly DME production with CO<sub>2</sub> vented. For the once-through design with CO<sub>2</sub> captured separately from H<sub>2</sub>S, the DME cost is 15 % higher than for the least costly DME with CO<sub>2</sub> vented. Remarkably, in the case when CO<sub>2</sub> and H<sub>2</sub>S are captured and piped together for underground storage, there is a cost reduction relative to the least costly DME with CO<sub>2</sub> vented. This result stems from the considerably simplified sulfur capture system (including elimination of the Claus and SCOT units) when H<sub>2</sub>S does not need to be captured separately from CO<sub>2</sub>.

Considering DME as a domestic cooking fuel, cost comparisons with LPG are appropriate. The LPG-equivalent costs for DME estimated in this paper range from \$ 399/t to \$ 437/t when CO<sub>2</sub> is vented and from \$ 380/t to \$ 478/t when CO<sub>2</sub> is captured and stored. The typical ex-refinery wholesale price of LPG at Chinese refineries in April 2003 averaged \$ 383/t. For further comparison, the health damage costs because of smoke from cooking with solid fuels in rural Chinese homes is estimated to be \$ 470 to \$ 2900 per t of LPG-equivalent cooking fuel (e.g., DME) that would be needed if all cooking energy needs of rural residents using solid fuels were to be met by DME or LPG.

Considering DME as compression-ignition engine automotive fuel, for which the engine efficiency advantage over a conventional gasoline engine is an estimated 18.5 %, the DME production cost is \$ 0.23- 0.26/l gasoline-equivalent in cases when CO<sub>2</sub> is vented and \$ 0.22- 0.28/l gasoline-equivalent when CO<sub>2</sub> is captured and stored. This suggests that DME vehicles could be competitive replacements for gasoline engine vehicles with only modest world oil prices (\$ 23/bbl or more), even with carbon capture.

The cost comparisons made for ICL-based methanol and DME in this paper would be more favorable if Chinese manufacturing, engineering, construction, and operation were used in developing the cost estimates. Various sources indicate capital costs for Chinese manufacturing and construction will be 60 % to 75 % of those estimated for US conditions.

Because of the high carbon content of coal per unit of energy, transportation fuels produced by ICL will lead to increased carbon emissions to the atmosphere compared to the use of petroleum-derived fuels if carbon capture and storage are not included as part of the ICL plant design. For example, with no CO<sub>2</sub> storage, the carbon emissions charged to methanol with recycle-based production would be 154 % of petroleum-gasoline emissions, even after considering the efficiency benefits of

methanol engines. With once-through methanol production, the carbon penalty is half of the penalty in the RC case or less.

When CO<sub>2</sub> capture/storage is introduced, carbon emissions will be less than carbon emissions from petroleum fuels and stand-alone electricity plants in most cases. For example, emissions charged to methanol are 75-81 % of petroleum emissions for RC-based methanol production and 56-72 % for OT-based production. ■

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#### Notes

- The proposed plant will use Shell gasification technology and SASOL Fischer-Tropsch synthesis technology to convert anthracite wastes (residues of coal mining) into 5000 barrels per day (bpd) of synthetic diesel, naphtha, and kerosene fuels, while co-producing 35 MW of electricity (1 barrel or bbl = 136.4 kg).
- China produced 3.3 million tonnes (Mt) of methanol in 2001 (the bulk from coal) and has announced at least 3 new coal-to-methanol projects, including a 0.6 Mt/yr facility at Jincheng Coal Mining Co. (Shanxi Province), a 0.3 Mt/yr facility at Zhongyuan Chemical Co. (Henan Province), and a 0.24 Mt/yr facility at the Yankuang Lunan Chemical and Fertilizer Co., in Yanzhou (Shandong Province).
- The fraction of CO<sub>2</sub> plus H<sub>2</sub>O in the feed gas to a methanol or DME synthesis reactor should be 2 % or higher [Moore, 2003].
- For methanol production with recycling, a steam-Rankine cycle was used in place of a combined cycle because of the low flow of the purge gas available to the power island. If a gas turbine were used, the exhaust heat would not be sufficient to provide the needed pre-heating of the synthesis cooling water to the required saturated condition. For DME production with recycling, some syngas was by-passed around the synthesis reactor to augment the purge gas flow to enable a gas turbine combined cycle to be used and sufficient electricity to be generated to meet the process needs.
- The fraction of methanol required to increase gasoline octane from 90 to 93 is determined by solving the following equation for x [Wyman et al., 1993]:  $93 = 90(1-x) + 120x$ . The value of the added methanol (in \$/l) is:  $P_{90} \times \{1 + [(P_{93}-P_{90})/P_{90}]x\}$ , where  $P_{90}$  and  $P_{93}$  are the wholesale prices of 90- and 93-octane gasoline (in \$/l).
- The sale price to resellers (who then sell to end-users) reflects gasoline production costs more closely than do sale prices to end-users.
- The total exposed population was estimated to be 109 million people [World Bank, 1997]. On the basis of annual per-capita liquid or gas fuel required for cooking, this exposed population would consume 174 to 371 million GJ/yr of clean cooking fuel (3.7-8.0 Mt/yr LPG, or 6.0-12.8 Mt/yr DME).
- The high cetane number of DME helps overcome cold-start difficulties, which today contribute to limiting the use of compression-ignition engines in many temperate regions to all but high-utilization-factor vehicles (buses, trucks).

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