A comparison of direct and indirect liquefaction technologies for making fluid fuels from coal

Robert H. Williams and Eric D. Larson
Princeton Environmental Institute, Princeton University
Guyot Hall, Washington Road, Princeton, NJ 08544-1003, USA
E-mail (Williams): rwilliam@princeton.edu

Direct and indirect liquefaction technologies for making synthetic liquid fuels from coal are compared. It is shown that although direct liquefaction conversion processes might be more energy-efficient, overall system efficiencies for direct and indirect liquefaction are typically comparable if end-use as well as production efficiencies are taken into account. It is shown that some synfuels derived via indirect liquefaction can outperform fuels derived from crude oil with regard to both air-pollutant and greenhouse-gas emissions, but direct liquefaction-derived synfuels cannot. Deployment now of some indirect liquefaction technologies could put coal on a track consistent with later addressing severe climate and other environmental constraints without having to abandon coal for energy, but deploying direct liquefaction technologies cannot. And finally, there are much stronger supporting technological infrastructures for indirect than for direct liquefaction technologies. Prospective costs in China for some indirect liquefaction-derived fuels are developed but not costs for direct liquefaction-based synfuels, because experience with the latter is inadequate for making meaningful cost projections. Especially promising is the outlook for the indirect liquefaction product dimethyl ether, a versatile and clean fuel that could probably be produced in China at costs competitive with crude oil-derived liquid fuels. An important finding is the potential for realizing, in the case of dimethyl ether, significant reductions in greenhouse gas emissions relative to crude oil-derived hydrocarbon fuels, even in the absence of an explicit climate change mitigation policy, when this fuel is co-produced with electricity. But this finding depends on the viability of underground storage of H_2S and CO_2 as an acid gas management strategy for synfuel production. Many "megascale" demonstration projects for underground CO_2 storage and H_2S/CO_2 co-storage, along with appropriate monitoring, modeling, and scientific experiments, in alternative geological contexts, are needed to verify this prospect. It is very likely that China has some of the least-costly CO_2 sources in the world for possible use in such demonstrations. It would be worthwhile to explore whether there are interesting prospective demonstration sites near one or more of these sources and to see if other countries might work with China in exploiting demonstration opportunities at such sites.

1. Introduction

China, with its rapidly growing demand for transportation fuels, scant domestic oil and natural gas resources but abundant coal, is likely to turn to coal as a basis for providing synthetic fluid fuels for transportation, cooking, and other applications that are not easily served by electricity.

Two very different approaches to providing fluid fuels from coal are described and compared in this paper: direct coal liquefaction (DCL) and indirect coal liquefaction (ICL). For both approaches a major challenge is to increase the hydrogen-carbon ratio. For finished hydrocarbon fuels such as gasoline and diesel, H/C ~ 2 (molar basis). For petroleum crude oil, the ratio ranges from 1.3 to 1.9. For typical bituminous coals, H/C ~ 0.8.

Making a comparison of DCL and ICL technologies is not an easy task because of the very different stages of development for these two classes of technologies. ICL technologies (Fischer-Tropsch (F-T) liquids, methanol (CH_3OH or MeOH) and dimethyl ether (CH_3OCH_3 or DME)) are either commercially proven or made up of proven modules, and there is an extensive literature on these technologies and modules. In contrast, DCL technologies are not yet commercially proven, and information available in the public domain is limited – with quite different findings coming from the few assessments that have been made. Despite this difficulty, enough is known about DCL technologies to offer policy-makers guidance in understanding the fundamental distinguishing aspects of these two classes of coal conversion technologies.

DCL technology involves making a partially refined synthetic crude oil from coal, which is then further refined

into synthetic gasoline and diesel as well as LPG – hydrocarbon fuel products similar to hydrocarbon fuels derived from petroleum crude oil.

ICL technology involves first gasifying coal to make synthesis gas ("syngas", mainly carbon monoxide (CO) and hydrogen (H_2)) and then making synthetic fuels from this syngas; the label "indirect" refers to the intermediate step of first making syngas. ICL technology can also provide hydrocarbon fuels that resemble crude oil-derived products. One possibility is synthetic middle distillates derived via the F-T process that can either be used directly as diesel or in blends with petroleum-derived diesel. Another possibility is gasoline via the route of first making MeOH from syngas and then converting MeOH into gasoline via the Mobil process. But MeOH can also be used directly as a fuel, and other oxygenates (fuels containing some oxygen) such as DME can also be provided via ICL process technology and used directly as fuels.
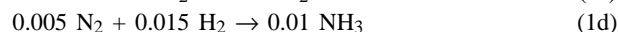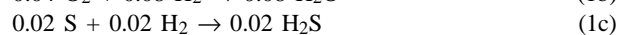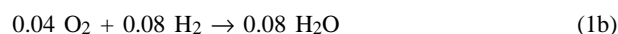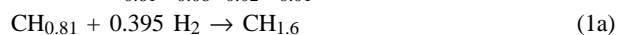
Making conventional hydrocarbon fuels from coal via either DCL or ICL processes has the advantage that the fuel infrastructures already in place for petroleum crude oil products can be used unchanged when a shift is made to coal-derived fuels. However, prospective air-pollutant regulatory constraints worldwide give high value to clean synthetic fuels with emission characteristics superior to those for petroleum crude oil-derived fuels. Moreover, the oft-cited advantage of fuel infrastructure compatibility offered by synthetic hydrocarbon fuels is not so great in China at present, where a liquid hydrocarbon fuel infrastructure for transportation fuels is at an embryonic state of development. For these reasons and because some oxygenates offer performance and emission characteristics superior to those for hydrocarbon fuels, the focus of ICL analysis in this paper is on the oxygenates MeOH and DME.

1.1. Direct coal liquefaction

With DCL technology the H/C ratio is increased by adding gaseous H_2 to a slurry of pulverized coal and recycled coal-derived liquids in the presence of suitable catalysts to produce synthetic crude oil. A slate of partially refined gasoline-like and diesel-like products, as well as propane and butane, are recovered from the synthetic crude oil mainly by distillation. Each of the products is made up of not one but many different large molecules that are recovered via distillation in different temperature "cuts".

Hydrogen is needed in the DCL process both to make synthetic crude oil (which might be represented in a simplified manner as $CH_{1.6}$) and to reduce the oxygen, sulfur, and nitrogen in the coal feedstock. These elements are removed from the liquid fuel products in the forms of H_2O, H_2S, and NH_3. The oxygen is removed so that hydrocarbon fuels can be obtained. The nitrogen and sulfur compounds are removed because they would otherwise poison the cracking catalysts in the refining operations downstream of the DCL plant.

The amount of H_2 needed is crudely estimated as follows for Yanzhou bituminous coal[1], which can be represented as $CH_{0.81}O_{0.08}S_{0.02}N_{0.01}$:

$$CH_{0.81} + 0.395 H_2 \rightarrow CH_{1.6} \tag{1a}$$

$$0.04 O_2 + 0.08 H_2 \rightarrow 0.08 H_2O \tag{1b}$$
$$0.02 S + 0.02 H_2 \rightarrow 0.02 H_2S \tag{1c}$$
$$0.005 N_2 + 0.015 H_2 \rightarrow 0.01 NH_3 \tag{1d}$$

Thus 0.5 kmol (1.0 kg) of H_2 plus 1 kmol (14.9 kg) of coal are required to produce 1 kmol (13.6 kg) of synthetic crude oil. The H_2 might be made from natural gas via steam reforming or from coal via gasification; the latter is a suitable option for China, where natural gas is scarce.

The DCL products are only partially refined. They must be further refined into finished liquid fuel products at conventional refineries, where additional H_2 is added (to bring the H/C up to ~ 2 for the final products), and energy is consumed to provide the refinery's heat and power needs.

DCL technology was invented by Friedrich Bergius in 1913 and commercialized in Germany and England in time to provide liquid fuels for World War II. The activity was abandoned when low-cost Middle East oil became available in the early 1950s. R&D was revived in the United States, Germany, and Japan after the Arab oil embargo of 1973. Interest in DCL declined again in the mid-1980s with the decline of the world oil price. None of the industrialized countries are now pursuing DCL technology to meet their own liquid fuel needs. Most global interest in alternatives to crude oil is focused on gas-to-liquids (GTL) technology, which aims to exploit low-cost "stranded" natural gas resources in various parts of the world. However, the Clean Coal Technology Program of the US Department of Energy is pursuing several projects that involve liquid fuel production via indirect coal liquefaction (ICL).

Modern DCL technology is not proven at commercial scale. The largest scale at which there has been experience with DCL in the United States is a Process Development Unit at the Hydrocarbon Technology, Inc. (HTI) R&D facility that consumes 3 tonnes (t) of coal per day.

In 2002, China announced a $ 2 billion investment for a DCL plant in Inner Mongolia based on HTI technology. The plant was expected ultimately to produce 50,000 barrels per day (b/d) (1 barrel = 0.1364 t) of partially refined gasoline and diesel and was to be made up of three reactor trains, each processing 4,300 t of coal daily. The first reactor train, which represents a scale-up by a factor of 1400 from the previous largest plant, was to start up in 2005. However, as this article was going to press in early December 2003, it was announced that construction of the plant is being suspended. The future of the project is now uncertain, but at the very least the project will be scaled down and its timing stretched out.

1.2. Indirect coal liquefaction

The first step in indirect liquefaction is to gasify coal in oxygen (partial oxidation) to produce syngas. The CO and H_2 molecules in the syngas are then combined catalytically to produce compounds that can be used as fuels – either hydrocarbon fuels such as synthetic gasoline or synthetic diesel, or oxygenated fuels. The challenge of increasing the H/C ratio is addressed by using the water-gas-shift (WGS) reaction ($CO + H_2O \rightarrow H_2 + CO_2$) and removing the CO_2 thereby produced from the system.

At present the most important options are hydrocarbon fuels synthesized via the F-T process, MeOH, and DME.

1.2.1. Fischer-Tropsch liquids

The F-T process for making synthetic hydrocarbons can be summarized, in a simplified manner, by the following two catalytic reactions that build up large hydrocarbon molecules from the small CO and H_2 molecules produced by gasification, with the oxygen in the CO feed being rejected in steam:

$$n\ CO + 2n\ H_2 \rightarrow n\ H_2O + C_nH_{2n}\ \text{(olefins)} \qquad (2a)$$
$$n\ CO + (2n + 1)\ H_2 \rightarrow n\ H_2O + C_nH_{2n+2}\ \text{(paraffins)} \qquad (2b)$$
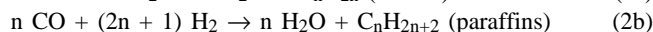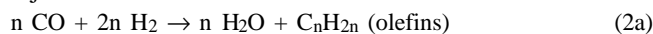
The slate of products generated depends on the catalysts used and reactor operating conditions. Olefin-rich products with n in the range 5 to 10 (naphtha) can be used for making synthetic gasoline and chemicals in high-temperature F-T processes. Paraffin-rich products with n in the range 12 to 19 (distillates) are well suited for making synthetic diesel and/or waxes in low-temperature F-T processes. Development has emphasized making synthetic diesel because the raw distillate product is an excellent diesel fuel, whereas the raw naphtha product requires substantial subsequent refining to make an acceptable gasoline.

F-T technology is well established commercially and is the focus of global GTL efforts to exploit low-cost "stranded" natural gas to make synthetic liquid transportation fuels. Sasol in South Africa has extensive construction and operating experience with F-T technology based on coal gasificaton and converts annually about 42 million t (Mt) of coal into 6 billion liters (Gl) of synthetic fuels and 2 Gl of chemicals [Geertsema, 1996]. And there is growing interest in coal-based F-T technology in the United States. Sasol F-T synthesis technology along with a Shell gasifier will be used in a $ 0.6 billion US Department of Energy-sponsored demonstration project in Gilberton, Pennsylvania, that will make from coal waste materials 5,000 b/d of F-T liquids plus 41 MW$_e$ of electricity. Recently, a detailed assessment was carried out for the US Department of Energy of the co-production of F-T liquids and electricity from coal via gasification at large scales [Bechtel et al., 2003a; 2003b]. This study, based on the E-Gas gasifier (now owned by PhillipsConoco) and slurry-phase reactors for F-T liquids synthesis, estimated that for an optimized plant[2] built in the US Midwest, the internal rate of return would be 10 % if the electricity were sold for $ 0.04/kWh and the F-T liquids for $ 30 per barrel; the equivalent crude oil price would be up to $ 10 per barrel less than this $ 30 per barrel cost (depending on refinery configuration and relative oil product demands), because the F-T liquids would already be partly refined [Marano et al., 1994].

Sulfur and aromatic-free F-T middle distillates are already being used as blend stock with conventional crude oil-derived diesel in California to provide fuel that meets that state's stringent specifications for diesel.

1.2.2. Methanol

MeOH is a well-established chemical commodity used throughout the world. It can potentially also be used indirectly or directly (see Box 1) as a fuel.

Box 1. MeOH as a synthetic fuel for transportation

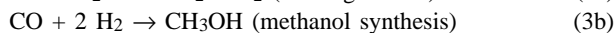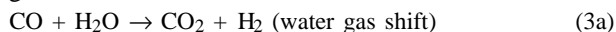Because of its high octane rating[28], MeOH is well-suited for use in SIE vehicles (see discussion in main text)[29]. It can be used in such vehicles with relatively modest modifications of the basic vehicle.

Used in SIE vehicles, MeOH offers air-quality benefits that are thought to be comparable to those offered by reformulated gasoline [Calvert et al., 1993]. The ozone formation potential from formaldehyde emissions of MeOH is thought to be less than the ozone formation potential of unburned hydrocarbon emissions; NO$_x$ emissions from MeOH engines operated at the same compression ratio as for gasoline would be less than for gasoline, because of the lower flame temperature, but when the compression ratio is increased to take advantage of MeOH's higher octane rating, thereby improving engine efficiency, this advantage may be lost [Wyman et al., 1993]. And just as some of the unburned hydrocarbon emissions for gasoline are carcinogenic, the US Environmental Protection Agency has classified formaldehyde as a probable human carcinogen, on the basis of evidence in humans and in rats, mice, hamsters, and monkeys [EPA, 1987].

The major drawbacks of MeOH as a transport fuel are its low volumetric energy density (half that of gasoline – see Table 4), its affinity for water, its corrosiveness, and its toxicity – a fatal dose is 2-7 % MeOH in 1 litre (l) of water, which would defy detection by taste.

Drawing upon HEI [1987] and Malcom Pirnie [1999], the following provides a perspective on the MeOH toxicity issue: MeOH is classified as a poison (it is rated as slightly more toxic than gasoline), and it is infinitely miscible with water (forms mixtures in all concentrations), allowing ready transport in the environment. Chronic low-dose MeOH vapor exposure from normal vehicle operations is not likely to cause health problems. However, exposure through MeOH-contaminated drinking water is a concern. In the event of a spill, MeOH would probably be less likely to reach drinking water supplies than gasoline, because natural processes would degrade it more quickly, but if MeOH-contaminated drinking water had to be treated (which it might if an underground MeOH tank leaked into groundwater), remediation would be more difficult than with gasoline.

The primary reactions involved in making MeOH from syngas are:

$$CO + H_2O \rightarrow CO_2 + H_2\ \text{(water gas shift)} \qquad (3a)$$
$$CO + 2\ H_2 \rightarrow CH_3OH\ \text{(methanol synthesis)} \qquad (3b)$$

The MeOH produced can be further processed to make gasoline by the Mobil process (a commercial technology that can provide gasoline at attractive costs from low-cost stranded natural gas [Tabak, 2003]) or DME by MeOH dehydration (see below), or the MeOH can be used

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Box 2. Dimethyl ether as a synthetic fuel

Dimethyl ether (DME) is a clean oxygenated synthetic fuel that can be made from any carbonaceous feedstock. It is a gas at ambient conditions but can be stored as a liquid in mildly pressurized canisters like those used for liquefied petroleum gas (LPG), a propane/butane mixture[30]. As a liquid DME's volumetric energy density (MJ/l) is 82 % of that for propane and 55 % of that for No. 2 diesel (see Table 4). DME is well suited for use as a transport fuel (as an alternative to diesel) as discussed in the main text, as a cooking fuel (as an alternative to LPG), and as a fuel for stationary power.

DME can be substituted for LPG, currently the preferred clean cooking fuel in rural areas where it is available and affordable and in urban areas where natural gas is not available. The demand for LPG in China has been growing rapidly [WLPGA, 2002]: from 2.54 Mt in 1991 (1.7 % of global production) to 14.2 Mt in 2001 (7.0 % of global production) – at an average rate of 19 %/year. It is unlikely that global LPG supplies would be adequate to satisfy the ultimate demand for clean cooking fuel in China – but DME produced from domestic energy resources in China would not be resource-constrained. Researchers at the Institute of Coal Chemistry of the Chinese Academy of Sciences have investigated prospects for making DME from coal for cooking applications [Niu, 2000]. For such applications DME's combustion properties are similar to those for LPG, though DME combustion generates less CO and hydrocarbon air pollution and DME is safer to use. An important consideration is that the infrastructure already established for LPG in China (and other developing countries) can be adapted, essentially without modification, to DME.

Because of its outstanding features as a fuel for compression-ignition engines (see main text), DME might also be used to produce electricity for rural areas in diesel engine/generator sets at scales of hundreds of kW (perhaps providing electricity more reliably than grid electricity in many instances), using the same DME infrastructure used to provide DME as a cooking fuel for such villages.

DME can also be used as a fuel for providing peaking and load-following power in modern gas turbines and gas turbine/steam turbine combined cycles. Use of DME for central station power generation in combined cycles is proven technology, for which emissions are as low as for natural gas combined cycles [Basu et al., 2001].

In the longer term, DME could also be used in low-temperature fuel cells either for transportation or in small-scale stationary power generating units. For such applications DME is relatively easy to reform – even easier to reform than MeOH[31].

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directly as fuel. This last option is the focus of the present study (see also companion paper in this issue by Larson and Ren [2003]).
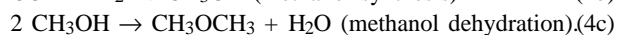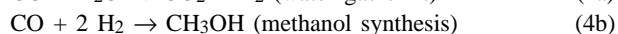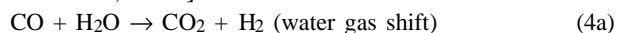
In most parts of the world MeOH is made by steam reforming of natural gas, but in gas-poor regions such as China it is made mainly from coal-derived syngas via gasification.

Under the US Department of Energy's Clean Coal Technology Program, Air Products and Chemicals, Inc., has brought to commercial readiness slurry-phase reactor technology for MeOH production [Heydorn et al., 2003]. Following successful proof-of-concept in 7,400 hours of test operation at a scale of 12,000 l/day at the DOE-owned process development unit at LaPorte, Texas, the technology has been demonstrated successfully at near-commercial scale (300,000 l/day rated capacity) at the Eastman Chemical Company's coal gasification facility in Kingsport, Tennessee; during the 69-month demonstration program since start-up in April 1997 the plant availability averaged 97.5 %.

1.2.3. Dimethyl ether

DME is a non-carcinogenic and virtually non-toxic chemical produced at a rate of 143,000 t/year for chemical process uses and one significant final consumer market: as an aerosol propellant that replaced fluorinated hydrocarbons phased out because of concerns about ozone-layer damage[3]. It is also usable as a fuel (see Box 2).

Currently DME is made by MeOH dehydration: $2\ CH_3OH \rightarrow CH_3OCH_3 + H_2O$. But DME can also be made (prospectively at lower cost) in a single step by combining mainly three reactions in a single reactor [Larson and Ren, 2003]:

$$CO + H_2O \rightarrow CO_2 + H_2 \text{ (water gas shift)} \tag{4a}$$
$$CO + 2\ H_2 \rightarrow CH_3OH \text{ (methanol synthesis)} \tag{4b}$$
$$2\ CH_3OH \rightarrow CH_3OCH_3 + H_2O \text{ (methanol dehydration)}. \tag{4c}$$

Haldor Topsoe in Denmark [Bøgild-Hansen et al., 1995; 1997] is developing a single-step process for making DME from natural gas. NKK Corporation in Japan [Ohno, 1999; Adachi et al., 2000] and Air Products and Chemicals, Inc., in the United States [Peng et al., 1997; APCI, 2002; Heydorn et al., 2003] are developing single-step processes for large-scale DME manufacture from coal-derived syngas using slurry-phase reactors.

In China, the Institute of Coal Chemistry (ICC) of the Chinese Academy of Sciences together with the Shanxi New Style Fuel and Stove Company constructed a 500 t/year DME plant in Xi'an based on MeOH dehydration for use as a domestic cooking fuel as an alternative to LPG (see Box 2); also, since 1995, the ICC has been carrying out R&D on one-step DME synthesis based on slurry-phase reactor technology [Niu, 2000].

The Ningxia Petrochemical Industry Lingzhou Group, Ltd., is pursuing plans to build a 830,000 t/year DME production plant in Lingwu City, Ningxia Province, based on use of a Chevron-Texaco coal gasifier and the slurry-phase reactor technology of Air Products and Chemicals, Inc. [Lucas and Associates, 2002]. The proposed plant would be built in two phases: during the first phase a 210,000 t/year plant would be built with a single gasifier

train; this would be followed in the second phase by the construction of a plant producing 620,000 t/year that would involve using three additional gasifier trains. In November 2001, the State Development Planning Commission gave tentative approval to the project. A detailed engineering feasibility study is being planned [Lucas, 2003], and efforts are on-going to find equity investors.

2. Comparative analysis

In this study a comparison is made of DCL and ICL technologies, with a focus on MeOH and DME as representative products of ICL, with respect to:

- system energy efficiency;
- air quality issues;
- GHG emission characteristics;
- suitability for transition to a highly decarbonized coal energy future; and
- supporting technological infrastructures.

Because DCL technologies, unlike ICL technologies, have not been demonstrated at near-commercial scales, a rigorous comparison of DCL and ICL fuel costs is not presently feasible. However, ICL technologies are sufficiently advanced that rough estimates of ICL fuel costs relative to costs for crude oil-derived fuels can be made for both US-built and China-built plants.

This study draws on detailed systems analyses for MeOH and DME carried out in Larson and Ren [2003], whereas the analysis of DCL technology is based on a literature review. Some characteristics of DCL production technologies are summarized in Tables 1a and 1b, while some characteristics of MeOH and DME production technologies are summarized in Tables 2a and 2b.

2.1. System energy efficiency

It is widely believed that making liquid fuels via DCL is more energy-efficient than via ICL. However, a comparison of conversion efficiencies at energy production facilities in isolation from other features of the fuels can be misleading. Moreover, because coal is an abundant, low-cost energy feedstock (compared to oil and natural gas), energy production conversion efficiency per se is not an especially important performance measure.

Table 1a presents estimates based on mid-1990s analysis by the developer of the HTI technology that coal liquids could be produced from coal at an overall efficiency of about 73 %[4]. Another analysis of HTI technology carried out then by a Bechtel/Amoco analytic team estimated a 58 % efficiency[5]. For comparison, the efficiencies for making MeOH and DME in dedicated plants (options labeled RC-V in Tables 2a and 2b) are 58.3 % and 55.1 %, respectively. Thus DCL and ICL conversion efficiencies would be similar if the Bechtel/Amoco estimate proves to be closer to realizable DCL efficiencies, but not if the HTI estimate proves to be closer to the mark.

But caution must be exercised in making such efficiency comparisons because DCL efficiencies are for partially refined products and ICL efficiencies are for making final products, and some ICL-derived products can be used at greater energy efficiency at the point of end-use than the products derived via refining from DCL.

Table 1a. Energy/ material balances for production of direct coal liquids – based on HTI estimates[1] (HHV basis)

	HTI design[1]	HTI design modified so that all H_2 made from coal
Energy inputs, 10^3 GJ/day		
Coal	257.9	354.7
Natural gas	94.4	-
Total	352.4	354.7
H_2 production, 10^5 kg/day		
From coal	3.02	7.90[2]
From natural gas	4.88[2]	-
Total	7.90	7.90
Energy outputs, 10^3 GJ/day (10^3 barrels/day)		
Gasoline (@ 5.84 GJ/barrel)	69.0 (11.8)	
Diesel (@ 6.08 GJ/barrel)	174.1 (28.6)	
Propane (@ 4.05 GJ/barrel)	13.2 (3.3)	
Butane (@ 4.62 GJ/barrel)	8.8 (1.9)	
Total (@ 5.81 GJ/barrel)	265.0 (45.6)	
Overall efficiency (%)	75.2	74.7
Fuel-cycle GHG emissions for final product		
In kg C/GJ of final product[3]	34.61	38.51
Relative to petroleum-derived gasoline[4]	1.45	1.61

Notes

1. An HTI design [Comolli et al., 1996] involves use of Wyoming coal from the Black Thunder Mine (27.10 MJ/kg (dry basis) or 28.83 MJ/kg (moisture-free and ash-free basis); carbon content = 25.81 kgC/GJ). The natural gas is assumed to have a carbon content of 13.95 kgC/GJ. All these energy values are on a HHV basis.

2. In the HTI design, 61.8 % of the needed H_2 is provided from natural gas via steam reforming. In shifting to the modified HTI design, it is assumed that this H_2 is produced instead from extra coal on the basis of the process described in Table 5. Thus, producing 4.88×10^5 kg/day = 58.56×10^3 GJ/day (LHV basis) of H_2 from coal (assuming, from Table 5, an effective efficiency of 63.7 %) requires 91.9×10^3 GJ/day of coal or 96.8×10^3 GJ/day (HHV basis).

3. The total fuel-cycle GHG emission rate for coal is the sum of the emission rate from the coal's carbon content (25.81 kgC/GJ, HHV) plus the upstream emission rate (0.96 kgC/GJ, HHV – see Note 12 to main text). The total fuel-cycle GHG emission rate for natural gas is the sum of the emission rate from the natural gas's carbon content (13.95 kgC/GJ, HHV) plus the upstream emission rate (2.56 kgC/GJ, HHV -- see Note 12 to main text). To get the fuel-cycle emissions/GJ of product it is assumed further that the downstream refinery consumes coal to meet its heat and power needs at a rate equal to 10 % of the syncrude energy content. With this assumption, the total fuel-cycle emissions/GJ of final product are, for the HTI design:
= $[(257.9 \times 10^3$ GJ/d + $0.1 \times 265.0 \times 10^3$ GJ/d)$\times$(25.81 + 0.96) kgC/GJ + 94.4×10^3 GJ/d$\times$(13.95 + 2.56) kgC/GJ]/(265.0$\times 10^3$ GJ/d) = 34.61 kg C/GJ,
and, for the modified (all coal) HTI design:
= $[(354.7 \times 10^3$ GJ/d + $0.1 \times 265.0 \times 10^3$ GJ/d)$\times$(25.81 + 0.96) kgC/GJ]/(265.0$\times 10^3$ GJ/d) = 38.51 kg C/GJ with the modified HTI design (all coal input).

4. On the basis of the GREET model for typical US conditions, the fuel-cycle emission rate for gasoline is 25.56 kg C/GJ (LHV, see Table 4) or 23.93 kg C/GJ (HHV basis).

The refining of DCL-derived syncrude to make finished products requires energy inputs both for heat and power and for making additional H_2 for fuel hydrogenation. Notably, energy requirements for petroleum refining can be significant – e.g., the primary energy required for heat and power at US refineries amounted to 13.3 % of the heating value of the total inputs to the refineries in 1994

Table 1b. Energy and material balances for production of direct coal liquids – based on Bechtel/Amoco estimates[1] (HHV basis)

	Bechtel/Amoco design	Bechtel/Amoco design modified so that electricity made from coal[2]
Energy inputs, 10^3 GJ/day		
Coal	704.9	704.9 + (0.90 × 88.5 / 0.644) = 828.6
Natural gas	88.5	-
Total	793.4	828.6
Energy outputs, 10^3 GJ/day (10^3 barrels/day)		
Naphtha (@ 5.64 GJ/barrel)	104.5 (18.5)	
Light distillate (@ 6.15 GJ/barrel)	43.6 (7.1)	
Heavy distillate (@ 6.15 GJ/barrel)	171.6 (27.9)	
Gas oil (@ 6.70 GJ/barrel)	143.2 (21.4)	
Propane (@ 4.04 GJ/barrel)	15.7 (3.9)	
Butane (@ 4.50 GJ/barrel)	10.0 (2.2)	
Total (@ 5.95 GJ/barrel)	488.6 (81.0)	
Overall efficiency (%)	61.6	59.0
Fuel-cycle GHG emissions		
In kg C/GJ of final product[3]	41.20	44.48
Relative to petroleum-derived gasoline[4]	1.72	1.86

Notes

1. The Bechtel/Amoco design [Bechtel and Amoco, 1992; 1993a; 1993b; Kramer, 2003] involves use of Illinois No. 6 coal from the Burning Star mine (33.68 MJ/kg (moisture-free and ash-free basis); carbon content = 23.81 kgC/GJ). The natural gas is assumed to have a carbon content of 13.95 kgC/GJ. All these energy values are on a HHV basis.

2. In the Bechtel/Amoco design, natural gas provides some of the fuel required for providing on-site power generation in a combined cycle power plant. It is assumed for the modified design that this natural gas is replaced by syngas derived from coal, assuming that the syngas and natural gas are equivalent on a LHV basis. For the Texaco gasifier operated on Illinois bituminous coal, the ratio of the LHV of the syngas output to the HHV of the total coal input (including coal for electricity for O_2 manufacture) is estimated to be 0.644 [Simbeck et al., 1993]. For natural gas, the LHV = 0.90×HHV.

3. The fuel-cycle GHG emission rate for coal is the sum of the emission rate from the coal's carbon content (23.81 kgC/GJ) plus the upstream emission rate (0.96 kgC/GJ – see Note 12 to main text). The fuel-cycle GHG emission rate for natural gas is the sum of the emission rate from the natural gas's carbon content (13.95 kgC/GJ, HHV) plus the upstream emission rate (2.56 kgC/GJ – see Note 12 to main text). To get the fuel-cycle emissions/GJ of product it is assumed further that the downstream refinery consumes coal to meet its heat and power needs at a rate equal to 10 % of the syncrude energy content. Thus, the total fuel-cycle emissions/GJ of final product are, for the Bechtel/Amoco design = [(704.9×10^3 GJ/d + 0.1×488.6×10^3 GJ/d)×(23.81 + 0.96) kgC/GJ + 88.5×10^3 GJ/d×(13.95 + 2.56) kgC/GJ]/(488.6×10^3 GJ/d) = 41.20 kg C/GJ, and, for the modified (all coal) Bechtel/Amoco design = [(828.6×10^3 GJ/d + 0.1×488.6×10^3 GJ/d)×(23.81 + 0.96) kgC/GJ]/(488.6×10^3 GJ/d) = 44.48 kg C/GJ.

4. On the basis of the GREET model for typical US conditions, the fuel-cycle emission rate for gasoline is 25.56 kg C/GJ (LHV basis) or 23.93 kg C/GJ (HHV basis).

[EIA, 1997]. In contrast, if MeOH or DME were to become a major energy carrier, no further refining energy requirements would be required[6].

The additional energy for refining DCL products would be especially significant in making synthetic diesel for use in compression ignition engines (CIEs). Having a fuel suitable for use in CIEs is highly desirable because such engines can be made much more energy-efficient than spark-ignition engines (SIEs). Weiss et al. [2003] estimate that advanced (2020-vintage) diesel-fueled CIE cars would be 18.5 % more energy-efficient than equivalent gasoline-fueled SIE cars. Key to good fuel performance in a CIE is a high cetane number (see Box 3). Liquid fuels derived from coal via DCL have a high content of aromatics[7], which implies a low cetane number; typically the distillate cuts of coal liquids that are potentially suitable for use as diesel have cetane numbers less than 30 [Lowe et al., 1997], compared to 40-50 for typical petroleum crude oil-derived diesel fuels. The challenge posed by the low cetane number can be dealt with by additional hydrogenation -- but this would entail a substantial energy

penalty associated with providing the extra H_2. In contrast, DME offers excellent performance in CIEs – with a cetane number of about 60 [Fleisch et al., 1997].

Much of the high energy penalty associated with raising the cetane number could be avoided by blending DCL diesel with F-T-derived middle distillates (cetane number ~ 70). But then DCL would be strongly coupled to ICL technology, not an independent technological option.

To the extent efficiency is a meaningful performance parameter, account should be taken of the total energy requirements for the final service provided, such as propelling a motor vehicle. To illustrate the importance of efficiency at the point of end-use consider DCL vs. ICL technologies for making fuels for SIE cars – DCL-derived gasoline vs ICL-derived MeOH.

The high aromatic content makes it possible to achieve reasonably high octane (anti-knocking feature) for DCL-derived gasoline, which implies engine performance comparable to but not higher than for gasoline derived from petroleum crude oil. In contrast, MeOH has a higher octane rating than gasoline (see Box 1) that makes it feasible

Table 2a. Performances and costs for producing MeOH from coal in alternative configurations – US construction[1]

Configuration[2]	OT-V	OT-C/S	OT-CC/CS	RC-V	RC-C/S	RC-CC/CS
MeOH output (MW)	626.0	626.0	626.0	626.0	626.0	626.0
Net electric power output (MW)	625.4	582.5	577.4	5.1	- 12.4	- 14.4
Coal input (MW)	2747.2	2747.2	2747.2	1085	1085	1085
MeOH energy production as % of coal energy input	22.8	22.8	22.8	57.7	57.7	57.7
Effective efficiency[3] (%)	48.4	45.0	44.6	58.3	56.2	56.0
CO_2 storage rate:						
In t CO_2/hour	-	438.5	475.8	-	178.5	193.3
In kg C/GJ of MeOH (as % of MeOH carbon content[4])	-	53.1 (279)	57.6 (303)	-	21.6 (114)	23.4 (123)
CO_2 transport and storage cost[5] ($/t CO_2)	-	4.93	4.71	-	6.72	6.42
Total capital required, overnight construction ($10^6)	1305.2	1338.6	1178.3	548.9	567.5	496.8
Components of MeOH production cost[6] ($/GJ)						
Capital charge	13.53	13.88	12.22	5.69	5.88	5.15
Operation and maintenance	3.11	3.19	2.81	1.31	1.35	1.18
Coal input (for coal @ $1.0/GJ)	4.39	4.39	4.39	1.73	1.73	1.73
Electricity co-product credit (P_E = electricity value in $/kWh)	$-277.5 \times P_E$	$-258.5 \times P_E$	$-256.2 \times P_E$	$-2.26 \times P_E$	$+5.50 \times P_E$	$+6.39 \times P_E$
CO_2 disposal cost	-	0.96	0.99	-	0.53	0.55
Total MeOH production cost ($/GJ)	21.03 $-277.5 \times P_E$	22.42 $-258.5 \times P_E$	20.41 $-256.2 \times P_E$	8.73 $-2.26 \times P_E$	9.49 $+5.50 \times P_E$	8.61 $+6.39 \times P_E$
Total MeOH production cost ($/GJ) if P_E = $0.0429/kWh[7]	9.13	11.33	9.42	8.63	9.73	8.88
Total MeOH production cost ($/t) if P_E=$0.0429/kWh[7]	182	225	187	170	192	175
Break-even crude oil price ($/barrel) if 1 GJ MeOH is worth 1 GJ gasoline[8]	34.3	45.2	35.6	31.8	37.3	33.0
Fuel-cycle GHG emissions[9]						
Allocated to MeOH, in kgC of CO_2 equivalent/GJ (as % of emissions for crude oil-derived gasoline[10])	20.9 (81.8%)	21.0 (82.2%)	21.0 (82.2%)	44.9 (175.7%)	25.0 (97.8%)	23.4 (91.5%)
Allocated to electricity, in gC of CO_2 equivalent/kWh (as % of emissions for coal steam-electric plants with FGD[11])	338.7 (118.6%)	157.5 (55.2%)	141.3 (49.5%)	219.1 (76.7%)	219.1 (76.7%)	219.1 (76.7%)
Cost of GHG emissions avoided [9] ($/t C)	-	69	18	-	57	12
If 1 GJ MeOH is worth 1.15 GJ gasoline[12]:						
MeOH cost[13] ($/GJ of gasoline equivalent)	7.94	9.85	8.19	7.51	8.46	7.72
Break-even crude oil price[8] ($/barrel)	28.3	37.9	29.6	26.1	30.9	27.2
Fuel-cycle GHG emissions in kg C/GJ of gasoline equivalent[14] (as % of emissions for crude oil-derived gasoline[10])	18.2 (71.2%)	18.3 (71.6%)	18.3 (71.6%)	39.0 (152.6%)	21.7 (84.9%)	20.3 (79.4 %)

Notes

1. Based on Larson and Ren [2003].

2. OT = once-through; RC = recycle; V = CO_2 vented (recovered H_2S converted to elemental S; recovered CO_2 vented); C/S = CO_2 captured/stored (recovered H_2S converted to elemental sulfur; recovered CO_2 dried/compressed to 150 bar for transport to underground storage site); CC/CS = CO_2 co-captured/co-stored (H_2S and CO_2 recovered together, dried, compressed to 150 bar for transport to underground storage site).

3. See Note 13 to main text.

4. See Table 4.

5. The CO_2 disposal cost C_D (in $/t of CO_2) is calculated according to the methodology presented in Box 7.

6. See Box 5.

7. This is electricity cost for IGCC plant with CO_2 vented (see Table 2c).

8. See Box 8. The break-even crude oil price in $/barrel = 159 times break-even crude oil price in $/l.

9. See Appendix A.

10. See Table 4.

11. See Table 2c.

12. Spark-ignited engines optimized for MeOH can extract 1.15 times as much useful work from a GJ of fuel as can a spark-ignited engine operating on gasoline.

13. Cost in $/GJ of gasoline equivalent = (MeOH cost in $/GJ)/1.15.

14. Emissions/GJ of gasoline equivalent = (emissions/GJ of MeOH)/1.15.

Table 2b. Performances and costs for producing DME from coal in alternative configurations – US construction[1]

Configuration[2]	OT-V	OT-C/S	OT-CC/CS	RC-V	RC-C/S	RC-CC/CS
DME output (MW)	599.5	599.5	599.5	599.5	599.5	599.5
Net electric power output (MW)	552.0	531.4	526.2	- 1.0	- 12.7	- 14.7
Coal input (MW)	2413.0	2413.0	2413.0	1085	1085	1085
DME energy production as % of coal energy input	24.8	24.8	24.8	55.2	55.2	55.2
Effective efficiency[3] (%)	53.1	50.9	50.4	55.1	53.8	53.6
CO_2 removal rate:						
In t of CO_2/hour	-	211.1	243.8	-	119.5	134.2
In kg of C/GJ of DME (as % of DME carbon content[4])	-	26.7 (149)	30.8 (172)	-	15.1 (84)	17.0 (95)
CO_2 transport and storage cost[5] ($/t CO_2)	-	6.66	6.03	-	8.45	7.91
Total capital required, overnight construction (10^6)	1173.8	1195.2	1053.1	576.2	590.8	520.4
Components of DME production cost[6] ($/GJ)						
Capital charge	12.71	12.94	11.40	6.24	6.40	5.63
Operation and maintenance	2.92	2.97	2.62	1.43	1.47	1.30
Coal input (@ $1.0/GJ)	4.03	4.03	4.03	1.81	1.81	1.81
Electricity co-product credit (P_E = electricity value in $/kWh)	$-255.8 \times P_E$	$-246.2 \times P_E$	$-243.8 \times P_E$	$+0.46 \times P_E$	$+5.88 \times 5P_E$	$6.81 \times P_E$
CO_2 disposal cost	-	0.65	0.69	-	0.47	0.49
Total DME production cost ($/GJ)	19.66 $-255.8 \times P_E$	20.59 $-246.2 \times P_E$	18.74 $-243.8 \times P_E$	9.48 $+0.46 \times P_E$	10.15 $+5.88 \times P_E$	9.23 $+6.81 \times P_E$
Total DME production cost ($/GJ) if P_E = $0.0429/kWh[7]	8.69	10.03	8.28	9.50	10.40	9.52
Total DME production cost ($/t) if P_E = $0.0429/kWh[7]	247	286	236	271	296	271
Break-even crude oil price ($/barrel) if 1 GJ DME is worth 1 GJ diesel[8]	39.8	47.4	37.5	44.4	49.5	44.5
Fuel-cycle GHG emissions[9]						
Allocated to DME, in kgC of CO_2 equivalent/GJ (as % of emissions for crude oil-derived diesel[10])	20.2 (77.4 %)	20.3 (77.7 %)	20.3 (77.7 %)	47.5 (181.9 %)	33.6 (128.7 %)	31.9 (122.2 %)
Allocated to electricity, in gC of CO_2 equivalent/kWh (as % of emissions for coal steam-electric plants with FGD[11])	332.6 (116.5 %)	237.8 (83.3 %)	223.3 (78.2 %)	219.1 (76.7 %)	219.1 (76.7 %)	219.1 (76.7 %)
Cost of GHG emissions avoided[9] ($/t C)	-	55	-15	-	109	48
If 1 GJ of DME is worth 1.185 GJ gasoline[12]:						
DME cost[13] ($/GJ of gasoline equivalent)	7.33	8.46	6.99	8.02	8.78	8.04
Break-even crude oil price[8] ($/barrel)	25.3	30.9	23.5	28.7	32.5	28.8
Fuel-cycle GHG emissions in kg C/GJ of gasoline equivalent[14] (as % of emissions for crude oil-derived gasoline[10])	17.0 (66.5 %)	17.1 (66.9 %)	17.1 (66.9 %)	40.1 (156.9 %)	28.4 (111.1 %)	26.9 (105.2 %)

Notes

1. Based on Larson and Ren [2003].

2. OT = once-through; RC = recycle; V = CO_2 vented (recovered H_2S converted to elemental S; recovered CO_2 vented); C/S = CO_2 captured/stored (recovered H_2S converted to elemental sulfur; recovered CO_2 dried/compressed to 150 bar for transport to underground storage site); CC/CS = CO_2 co-captured/co-stored (H_2S and CO_2 recovered together, dried, compressed to 150 bar for transport to underground storage site).

3. See Note 13 to main text.

4. See Table 4.

5. The CO_2 disposal cost C_D (in $/t of CO_2) is calculated according to the methodology presented in Box 7.

6. See Box 5.

7. This is electricity cost for IGCC plant with CO_2 vented (see Table 2c).

8. See Box 8. The break-even crude oil price in $/barrel = 159 times break-even crude oil price in $/l.

9. See Appendix A.

10. See Table 4.

11. See Table 2c.

12. DME-fueled compression-ignited engines can extract 1.185 times as much useful work from a GJ of fuel as can a spark-ignited engine operating on gasoline.

13. Cost in $/GJ of gasoline equivalent = (DME cost in $/GJ)/1.185.

14. Emissions/GJ of gasoline equivalent = (emissions/GJ of DME)/1.185.

Table 2c. Performances and costs for generating electricity from coal with alternative technologies and at alternative sites

	Steam-electric plant constructed in China[1] with:		IGCC, with costs based on construction in			
	ESP	ESP + SO₂, NOₓ controls	China[2]	United States[3]		
Net electric power output (MWₑ)	300	300	390.1	390.1	361.9	361.9
Coal input (MW)	882	909	908.3	908.3	983.7	983.7
Efficiency (%)	34.0	33.0	43.0	43.0	36.8	36.8
SO_2 emission rate[4] (g/kWh)	33.3	3.4	0.26	0.26	0.31	0.31
NO_x emission rate (g/kWh)	3.0	1.2	0.087[5]	0.087[5]	0.102[5]	0.102[5]
CO_2 is	vented	vented	vented	vented	captured/ stored	co-captured/ co-stored
CO_2 emission rate from power plant[6] (g C/kWh)	266.5	274.6	210.8	210.8	21.5	21.5
Fuel-cycle GHG emission rate[6] (g C equivalent/kWh)	277.1	285.5	219.1	219.1	31.3	31.3
CO_2 removal rate[7] (t/hour)	-	-	-	-	298.1	298.1
CO_2 disposal cost ($/t CO_2)[8]	-	-	-	-	5.48	5.48
Specific capital required, overnight construction ($/kWₑ)	600	788	798	1202	1558	1425
Components of production cost (US¢/kWh)						
Capital charge (ACCR = 15 %/y, CF = 85 %, IDC = 0.16)	1.41	1.84	1.87	2.81	3.64	3.33
Operation and maintenance (4 % of total capital cost)	0.32	0.42	0.43	0.65	0.84	0.77
Coal input (for coal @ $1.0/GJ)	1.06	1.09	0.84	0.84	0.98	0.98
CO_2 disposal cost	-	-	-	-	0.45	0.45
Total production cost (US¢/kWh)	2.78	3.35	3.14	4.29	5.91	5.53
Cost of GHG emissions avoided ($/t C)[9]	-	-	-	-	86	66

Notes

1. From Wu et al. [2001] except O&M costs assumed to be 4 % of overnight capital cost, to be consistent with IGCC cost estimates of Kreutz et al. [2003].

2. It is estimated that the capital cost of an IGCC plant built in China is 0.664 times that of a plant constructed in the US (see Note 25 to main text).

3. Performances/costs based on Chiesa et al. [2003] and Kreutz et al. [2003] for US IGCC plant, except: (1) C/S contents of coal assumed to be those for Yanzhou bituminous coal (see Notes 4 and 6, this table) rather than Illinois No. 6 bituminous coal (assumed in those studies), and (2) coal price is assumed to be $1.0/GJ.

4. The assumed coal is high sulfur (3.69 % S) Yanzhou bituminous coal (23.494 GJ/t), so that the sulfur content = 1.57 kg S/GJ. The SO_2 emission rate is thus 33.25 g/kWh for coal steam-electric plants without SO_2 controls, 3.43 g/kWh for steam-electric plants with FGD (90 % S recovery), and 0.26 g/kWh for IGCC plants (99 % S recovery).

5. The NO_x emission rate for IGCC plants is assumed to be the measured rate achieved at the Buggenum IGCC plant, 10.44 g/GJ of coal [Van der Burgt, 1999].

6. The carbon content of Yanzhou bituminous coal is 25.174 kg C/GJ. The upstream GHG emission rate (CO_2 equivalent) is assumed to be 1.0 kgC/GJ.

7. Following Chiesa et al. [2003], 91.28 % of the carbon in the coal is recovered as CO_2.

8. The CO_2 disposal cost C_D (in $/t of CO_2) is calculated according to the methodology presented in Box 7.

9. Cost of avoided CO_2 emissions for an option that involves CO_2 capture = $(C_C - C_V)/(E_V - E_C)$, where C_C = electricity cost ($/kWh) for CO_2 capture option, C_V = cost ($/kWh) with CO_2 vented, E_C = GHG emissions (tC of CO_2 equivalent/kWh of electricity) for capture option, and E_V = GHG emissions (tC of CO_2 equivalent/kWh of electricity) when CO_2 is vented.

to design higher compression ratio engines that are 15-20 % more energy-efficient than gasoline engines [Grayson, 1984; Gray and Alson, 1989; Wyman et al., 1993]. If this potential end-use efficiency advantage (assumed to be 15 %) were exploited, the overall system efficiencies would be the same for ICL MeOH and DCL gasoline used in SIE vehicles if the losses from additional refining in the DCL case were about 8 %, assuming the HTI estimate of DCL conversion efficiency (73 %)[8].

2.2. Air quality issues

Consideration of the relative capabilities of DCL- and ICL-derived fuels for transportation in meeting air quality regulations is likely to figure prominently in assessments of the relative merits of these alternative routes to providing liquid fuels from coal.

2.2.1. Air quality regulatory trends

The historical trend in industrialized countries has been to tighter air-pollutant emission regulations over time, in response to both improving scientific understanding of damage caused by air pollution and growing public concerns about environmental quality with rising incomes. Table 3 illustrates the trend for US regulations of heavy-duty CIE vehicles, including the new Environmental Protection Agency (EPA) regulations for heavy-duty CIE vehicles that call for an order of magnitude reduction in both NO_x and particulate (PM) emissions by 2007.

Box 3. Cetane number for fuels used in compression ignition engines

The cetane number of a fuel is a measure of its tendency to auto-ignite and is related to the delay between start of fuel injection and start of combustion – the shorter the delay the higher the cetane number. A high propensity to self-ignite is undesirable for fuels used in SIEs (where a spark ignites the fuel at just the right time) but desirable for fuels used in CIEs.

A fuel with a high cetane number has numerous advantages [Edgar et al., 1995]:

"First, cold-start problems which plague many smaller automotive-type engines especially in cold climates can be reduced. This would eliminate the need for glow plugs, and potentially, the use of indirect injection engines which are inherently less efficient because of wall losses. Further, improving the cetane number of a fuel allows reliable ignition in an engine with lower compression ratio. Many engines today operate at compression ratios beyond the optimum for efficiency, because they must ensure the cylinder is adequately heated by compression to achieve good auto-ignition performance.

"Higher cetane numbers may also lead indirectly to lower NO_x emissions... A high cetane number fuel burns much more quickly upon injection, and eliminates the build-up of premixed zones that ignite suddenly, causing high pressure pulses and a concomitant increase in temperature which leads to the formation of NO_x via the thermal mechanism. In addition to eliminating the premixed burning, a high cetane number allows spark timing to be retarded, which decreases the amount of time NO_x forming gases are exposed to high temperatures...

"Finally, a high cetane fuel can reduce NO_x because it allows the engine to become more tolerant of EGR. EGR is proven to reduce NO_x in diesel engines by lowering combustion gas temperatures; however, it affects reliability of auto-ignition, and leads to an increase in smoke, carbon monoxide, and unburned hydrocarbon emissions. With a high cetane fuel ignition reliability can be maintained at high levels of EGR..."

Complying with these new regulations with diesel will require complicated and/or costly control technologies because conventional control measures for NO_x tend to cause higher PM emissions, and vice versa. The EPA recognized that it would not be feasible to satisfy the 2007 emission levels with the needed exhaust gas after-treatment technologies unless there were simultaneously a dramatic reduction in diesel's sulfur content – otherwise the sulfur would damage the exhaust gas after-treatment technologies. So the EPA simultaneously mandated that by 2007 diesel fuel must contain no more than 15 ppm sulfur (S), compared to 500 ppm S at present. Redesigning re-

fineries to meet this new regulation is now a major focus of US oil industry activity.

These tough regulations were motivated by powerful evidence that diesel emissions cause significant damage to public health, especially chronic mortality impacts of small air-pollutant particles that are either emitted directly from vehicles or are formed in the atmosphere from gaseous precursor emissions [EPA, 2001]. Meeting the 2007 standard will be a daunting challenge, requiring substantial investments in additional exhaust gas after-treatment technology, but diesel engine manufacturers are working intensely to have emission control technologies available on time and without incurring prohibitive cost penalties.

The trend in many developing countries has been to introduce air pollution regulatory policies similar to those already adopted in the industrialized countries – after a lag of several years. Indeed, historically, rapidly industrializing countries such as China, Taiwan, and Thailand have adopted tighter vehicle emission standards in just this manner [ADB, 2003]. Although the transport sector is relatively small in China at present, it is growing rapidly [Walsh, 2003], so that increasing attention is likely to be given to the public-health issues associated with air pollution for transportation as the sector expands. This attention will be buttressed by a growing affluence that is not only making this rapid growth possible but is also leading to higher public concerns about environment and public health issues – reflecting the well-known phenomenon that these concerns grow with per capita GDP.

2.2.2. Comparing air-pollutant emissions in transportation applications

DCL-derived and ICL-derived fuels have one common air quality advantage relative to petroleum crude oil-derived gasoline and diesel: a low S content that arises primarily as a result of process technology requirements – to protect cracking catalysts at the downstream refinery for DCL syncrude (as discussed above) and to protect synthesis reactor catalysts in making MeOH or DME (as discussed below). But aside from this common characteristic, emissions for DCL- and ICL-derived fuels will often differ markedly.

The authors are aware of no studies that have been carried out for motor vehicle air-pollutant emission characteristics for fuels derived from 100 % DCL syncrude. However, the Southwest Research Institute and Bechtel National have carried out engine tests and analyses for fuels derived from a conventional refinery that co-processes a mix of 37 % DCL synthetic crude and 63 % petroleum crude (see Box 4). The refinery products (regular gasoline, premium gasoline, and diesel with estimated syncrude contents of 49 %, 40 %, and 16 %, respectively (see Box 4)) were tested in engines with exhaust gas recirculation (EGR) via procedures that simulate real-world driving conditions. It was found for both gasoline and diesel that emissions were largely indistinguishable from emissions for cars and trucks fueled with petroleum crude oil-derived gasoline and diesel. The test results for heavy-duty CIEs operated on conventional petroleum crude oil-derived diesel and "partial coal-derived synthetic diesel"

are presented in Table 3, together with EPA emission standards for heavy-duty CIE vehicles. This table shows that for either fuel trucks would meet the EPA standard for PM through 2006 and the NO_x + NMHC (non-methane hydrocarbons) standard through 2003. Moreover, the latter standard for 2004-2006 would be exceeded by only 11 %. However, in both cases reductions of 84 % and 93 % for PM and NO_x, respectively, would have to be realized to meet 2007 standards.

Consider next DME used in CIE vehicles. Table 3 shows that, without exhaust after-treatment technology, NO_x and PM emissions are, respectively, 58 % and 75 % less for DME than for diesel; for DME with EGR, NO_x emissions are 74 % less than for an uncontrolled diesel engine and 63 % less than for a diesel engine with EGR – performance that is facilitated by DME's high cetane number (see Box 3). The low PM emissions arise as a result of the oxygen in the fuel (no C-C bonds that would lead to some soot formation). The low NO_x emissions arise in part from DME's high cetane number (see Box 3). Table 3 shows that for heavy-duty CIE vehicles, the US EPA standards through 2006 could be easily met with DME, without exhaust gas after-treatment. NO_x + NMHC emissions and PM emissions are, respectively, 24 % and 80 %[9] lower than the standard. The 2007 EPA standards could not be met without exhaust gas after-treatment, but the clean-up requirements are much less daunting than they would be for either conventional diesel or partial synthetic diesel derived from coal via DCL (see Table 3). This is both because the needed percentage emission reductions are much less, and also because low PM emissions are inherent in DME's chemical structure, so that the tradeoff between low NO_x emissions and low PM emissions that frustrates most traditional emission control strategies for diesel is absent for DME.

Also, according to Fleisch and Meurer [1995], engine tests indicate that a DME-fueled light-duty CIE passenger car (1360 kg inertia test weight) equipped with an oxidation catalyst has the potential to meet the California ULEV emission regulation – with quiet combustion. These features, along with DME's high cetane number, suggest a good potential for using DME in passenger cars as well as in heavy-duty CIE vehicles. And, as shown below, DME produced in polygeneration systems and used in cars could potentially be competitive in China with gasoline derived from crude oil at crude oil prices of $ 15-20 per barrel – even without taking credit in the cost calculations for the environmental benefits offered by DME.

In considering air quality issues relating to DCL and ICL fuels, it is desirable to look beyond the issues of the day discussed to this point and anticipate what other issues might emerge in the future, in the light of the historical trend toward ever tighter regulations and the long (5-20-year) planning time horizon for large synfuel plants. Late in the period between now and 2020 concerns of air quality regulators might be considerably greater than at present.

One potentially important consideration is the high aro-

Box 4. Air-pollutant emissions for synfuels derived from DCL/crude oil blends

In the late 1990s, the Southwest Research Institute and Bechtel National carried out tests and analyses in the United States for gasoline and diesel fuels derived from a conventional refinery that co-processes DCL synthetic crude and petroleum crude oils, using a linear programming refinery model [Lowe et al., 1997; Erwin et al., 1997; Southwest Research Institute and Bechtel National, 2001]. This modeling exercise (based on the DCL outputs presented in Table 1b) found that there was no economic optimum mix of syncrude and petroleum crude inputs but rather that as the syncrude fractional share of inputs increased, the syncrude value per barrel decreased, reflecting increasing processing costs per barrel because of constraints on unit capacities, feedstock specifications, utilities, etc. Accordingly, the study instead imposed a physical constraint on the system: the syncrude input share was constrained at the maximum (assuming zero value for coal liquids) that could be accommodated at an existing refinery with a fixed slate of products producing 150,000 barrels per day. Under this constraint the coal liquids input share was found to be 37 % on a volume basis. The estimated coal liquids fraction of the finished products turned out to be much higher for gasolines (49 % for regular, 40 % for premium) than for diesel (16 %), because the crude coal liquids contain a relatively high proportion of naphtha (gasoline feedstock), and because the refinery model selected the heavy distillate and gas oil cuts of the coal liquids to be catalytically cracked (primarily into gasoline blend-stocks); thus only the light distillate cut (see Table 1b) is available for making diesel, and this cut is also used for making jet fuel.

The gasoline from this refinery was then tested in a car with a SIE and advanced engine controls, and the diesel fuel was tested in a heavy-duty truck CIE equipped with exhaust gas recirculation. In both cases testing procedures that simulate real-world driving conditions were used. The test results for diesel heavy-duty CIE vehicles operated on both petroleum crude oil-derived diesel and "partial coal-derived synthetic diesel fuel" are presented in Table 3.

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matic content of DCL liquids. Despite the technical advantage this implies for making high-octane gasoline discussed above, the trend in environmental regulations in industrialized countries is to limit sharply the aromatic content of motor fuels. This trend was first manifest in the US in 1988, when the California Air Resources Board mandated that, beginning in 1993, motor vehicle diesel sold in California shall have an aromatic content no greater than 10 % (20 % for small refiners) -- a regulation aimed mainly at reducing emissions of both PM and NO_x for diesel use in California. Subsequently, the Clean Air

Table 3. US EPA emission standards and emissions from tests for alternative technologies, heavy-duty CIE road vehicles (g/bhp-hour)[1]

	HC[2]	NMHC + NOₓ[2]	NOₓ[2]	PM[2]
US EPA regulation[3]		-		
1990	1.3	-	6.0	0.60
1991	1.3	-	5.0	0.25
1993	1.3	-	5.0	0.25 (0.10 UB)
1994	1.3	-	5.0	0.10 (0.07 UB)
1996	1.3	-	5.0	0.10 (0.05 UB)
1998	1.3	-	4.0	0.10 (0.05 UB)
2004	-	2.4 (2.5 with 0.5 NMHC cap)	-	0.10 (0.05 UB)
2007	0.14 NMHC	-	0.20	0.01
Tests for turbocharged, intercooled, heavy-duty engine operated on:[4]				
Conventional diesel fuel (no exhaust gas after-treatment)	0.3	-	3.8	0.08
DME (no exhaust gas after-treatment)	0.3	-	1.6	0.02 (from lube oil)
DME (exhaust gas recirculation)	0.3	-	1.0	0.02 (from lube oil)
Tests for turbocharged heavy-duty engine with exhaust gas recirculation operated on:[5]				
Partial synthetic diesel fuel (a blend containing 15.9 % HTI light distillate (refined from a mix of 37.0 % DCL coal syncrude (HTI technology), 50.9 % petroleum crude oil, and 12.1 % MTBE, butanes, etc.)	0.149	-	2.63	0.063
Conventional diesel fuel derived from petroleum crude oil	0.152	-	2.68	0.068

Notes

1. bhp-hour = brake horsepower-hour. 1 g/bhp-hour = 1.34 g/kWh.

2. HC = hydrocarbons; NMHC = non-methane hydrocarbons; NOₓ = oxides of nitrogen (measured as NO_2); PM = particulate matter.

3. Based on EPA [1997] through 2004 and EPA [2001] for the 2007 regulations.

4. From Fleisch et al. [1997].

5. From SRI and Bechtel [2001]; see also Erwin et al. [1997] and Lowe et al. [1997].

Act Amendments of 1990 put sharp limits on the aromatic content of motor fuels generally in the United States. Although the benzene content of coal liquids is low, coal liquids have a high content of polycyclic aromatic hydrocarbons (PAHs), a class of organic compounds that include potent mutagenic and carcinogenic compounds [Nauss, 1995]. Motor vehicles account for about 1/3 of total US PAH emissions, and PAHs measured in urban air and roadway tunnels have been found in the respirable size range. Moreover, for light-duty vehicles (e.g., cars), PAH emission factors have been found to be correlated with PAH concentrations in gasoline [Marr et al., 1999]. The challenge posed by PAH can be dealt with by hydrogenation to reduce aromatics to naphthenes (ring compounds with only single carbon-carbon bonds), but this entails an energy penalty associated with providing the extra H_2.

Besides PAHs, coal also contains many toxic inorganic elements such as cadmium (Cd), arsenic (As), lead (Pb), selenium (Se), and mercury (Hg) that might be carried over into liquid fuel products. In the United States, Hg emissions from coal power plants are a focus of concern, and there are intense public debates as to whether Hg emissions ought to be regulated. If Hg were to become a major environmental concern, it would have to be removed in synfuels manufacture via both DCL and ICL processes. In all likelihood it would never be a significant issue for ICL processes, which start with gasificaton, because Hg removal via carbon filters is already proven technology for coal IGCC systems, and costs of removing ~ 99 % of Hg from syngas are trivial[10]. Such filters are effective in removing other toxic metals as well.

This discussion highlights a fundamental challenge posed by coal in the manufacture of liquid fuels: the fact that coal is made up of a large number of different substances, many of which are toxic or otherwise hazardous. In an ever-changing regulatory environment, the process of manufacturing fuels from coal via DCL processes would require continual adjustments in the technology and concomitant major investments to meet new regulatory mandates.

In contrast, ICL, which starts with the manufacture of syngas, represents a fundamentally different approach to synthetic fuels that makes it possible to: (1) establish a set of criteria for the "ideal" fuel with respect to performance, emissions, and cost, and search to see how close one can come to meeting the criteria with chemicals that can be manufactured from CO and H_2; and (2) choose for

Table 4. Some properties of alternative fuels

	Gasoline[1]	Diesel[1]	Methanol	DME	Propane	Butane
Chemical formula			CH_3OH	CH_3OCH_3	C_3H_8	C_4H_{10}
Molecular weight			32.043	46.069	44.096	58.123
Saturated vapor pressure @ 20ºC, bar				5.1	8.4	2.1
Liquid density @ 20ºC, kg/l	0.738	0.856	0.797	0.668	0.501	0.610
LHV, MJ/kg	42.58	41.68	19.9	28.5	46.4	45.7
LHV, MJ/l @ 20ºC	31.44	35.68	15.9	19.0	23.2	27.9
Carbon content, kgC/GJ	19.59	20.87	18.8	18.3	17.6	18.09
Fuel-cycle GHG emissions (CO_2 equivalent), kgC/GJ	25.56	26.11	-	-	-	-

Note

1. Source: US gasoline (reformulated with MTBE, 30 ppm S) and diesel (15 ppm S) derived from crude oil, from Argonne National Laboratory's GREET model.

focused development, from the many alternative options for combining CO and H_2 into fuel, those options that are vastly superior to conventional hydrocarbon fuels with regard to these criteria. In this development process eliminating ab initio the inherently noxious materials in coal from the syngas is not just an option: it is an essential part of the manufacturing process to protect synthesis reactor catalysts.

This approach to ICL technology might be called a "designer fuel strategy" for coal. It is fundamentally different from the DCL approach, which aims to make coal processing as much like petroleum crude oil processing as possible. Of course, not all ICL-derived synthetic fuels will be superior to petroleum-derived fuels – e.g., the air emissions and toxicity characteristics for MeOH are thought to be, on balance, about the same as for reformulated gasoline (see Box 1). But there are many possible fuels that might be manufactured via ICL, and some options, such as DME, seem to be markedly better than petroleum-derived fuels.

2.3. GHG emission characteristics

Synthetic fuel manufacture via either DCL or ICL technology can lead to large increases in greenhouse gas emissions relative to obtaining fuels derived from petroleum crude oil. However, there is scope for reducing GHG emissions somewhat without driving up synfuel costs substantially. In both cases streams of relatively pure CO_2 are generated as a result of the need to bring the H/C ratio up from the ~ 0.8 value for coal to a level in the range 2-4, depending on the synfuel being made. This CO_2 might be captured, dried, compressed, and transported to suitable sites for underground storage (see Box 6). Specific costs ($/kg CO_2) for fossil fuel decarbonization in this manner are far less than the costs of recovering CO_2 from flue gases of fossil fuel power plants or boilers, where the CO_2 stream is heavily diluted with nitrogen from combustion air, making CO_2 separation costs high [IPCC, 2003]. As will be shown: (1) there are substantial differences between DCL and ICL technologies with regard to the potential and costs for GHG emission mitigation; and (2) in the case of ICL (but not DCL)

Box 5. Methodology for energy cost calculations

Cost calculations for energy conversion are carried out under the following assumptions.
- Energy conversion facilities operate on average at 85 % of rated capacity.
- Costs are in constant 2002 US$ (exchange rate of 8.3 yuan RMB/$).
- Construction requires 4 years, during which time four equal annual payments are made for the capital cost, so that interest charges accumulated during construction amount to 16 % of the overnight construction cost (OCC), assuming a 10 % real interest rate.
- The annual capital charge rate applied to total capital is 15 % (corresponding to a charge rate of 1.16×15 = 17.4 % applied to the overnight construction construction cost).
- Annual operation and maintenance costs (in $/year) are assumed to be 4 % of the OCC.
- All energy quantities are presented on a lower heating value (LHV) basis unless explicitly indicated otherwise.
- The coal price = US$ 1.0/GJ (US$ 29.3 = 243 yuan RMB/t of coal equivalent (tce))

technologies there are even potentially significant GHG mitigation opportunities that could be pursued in the absence of an explicit climate mitigation policy.

In what follows GHG emission characteristics of DCL and ICL systems are described both without and with partial CO_2 capture/storage. Emissions from primary resource extraction through ultimate fuel use are considered – not just emissions from the synthetic fuel conversion facility. Fuel-cycle GHG emission rates for alternative synthetic fuels are compared to those for gasoline or diesel derived from petroleum crude oil, as appropriate, assuming the latter are low-sulfur gasoline or diesel[11], which might be characteristic of the situation in China by 2020, if the air-pollution regulatory situation in China at

Box 6. Geological disposal of CO_2

The relatively pure streams of CO_2 recovered as a natural by-product of the manufacture of H_2 (Table 5), MeOH (Table 2a), or DME (Table 2b) from coal can be either vented to the atmosphere or stored underground in alternative media: depleted oil and natural gas fields, deep beds of unminable coal, or deep saline aquifers [IPCC, 2003]. For the first two options CO_2 injection can sometimes be used for enhanced oil recovery, enhanced natural gas recovery, or enhanced coal-bed methane recovery [Gunter et al., 1997; Williams, 1999]. The technology is proven only for enhanced oil recovery. There are about 74 enhanced oil recovery (EOR) projects worldwide, mostly (66) in the United States, where in 2000 oil production via EOR reached 216,000 barrels per day (4 % of total US oil production), a by-product of which is the sequestration of 30 Mt of CO_2 annually. Most of the injected CO_2 comes from natural reservoirs of CO_2, but 5 Mt/year comes from anthropogenic waste CO_2 sources [Stevens et al., 2000].

Potential CO_2 storage opportunities are especially large for storage in deep saline aquifers, for which there are no enhanced resource recovery opportunities. Such aquifers are present in all sedimentary basins, the total area of which amounts to 70 million km^2 worldwide (two-thirds onshore and one-third offshore) – more than half of the 130 million km^2 of land area of the inhabited continents. To achieve high storage densities, CO_2 should be stored at supercritical pressures[32], which typically requires storage at depths greater than 800 m[33]. The aquifers at such depths are typically saline[34] and not effectively connected to the much shallower (depths less than ~ 300 m) freshwater aquifers used by people. Estimates of the global capacity for CO_2 storage in deep aquifers range from 2,700 GtC [Ormerod, 1994] to 13,000 GtC [Hendriks, 1994]. For comparison, estimated remaining recoverable fossil fuel resources (excluding methane hydrates) contain 6,000-7,000 GtC [Rogner, 2000].

One large aquifer storage project being carried out by Statoil involves separating CO_2 from the "sour" natural gas at the Sleipner Vest offshore natural gas field in Norway and injecting the CO_2 for storage into a nearby aquifer under the North Sea; CO_2 has been injected continuously into this aquifer at a rate of 1 Mt/year since 1996, and storage seems to be secure. Other large aquifer disposal projects are being planned.

that time is similar to that expected for the US in 2007 (see Table 3). Direct CO_2 emissions for coal vary from case to case, depending on the type of coal; direct emissions for natural gas are assumed to be 15.5 kg C/GJ (or 13.95 kgC/GJ, HHV). The emissions upstream of the coal and natural gas energy conversion facilities are assumed to be as estimated for typical large conversion plants in the United States at present[12].

2.3.1. DCL technologies

When all CO_2 generated at the conversion plant is vented to the atmosphere, fuel-cycle-wide GHG emissions for DCL-derived fuels are high compared to making fuels from crude oil, although there is considerable uncertainty regarding these emissions. Estimates range from 1.6 times the emission rate for gasoline, based on analysis of energy/material balances carried out for the US DOE by one developer of the technology (Table 1a), to 1.9 times the rate for gasoline, based on an analysis carried out for the US DOE by the Bechtel/Amoco group (see Table 1b).

The H_2 required to make DCL liquids in China would probably be made from coal via high pressure oxygen-blown gasification. Table 5 presents material and energy balances as well as costs for a typical modern coal-to-H_2 production plant. After gasification, the syngas is cooled and cleaned of particles. The cooled syngas is then reacted with steam in H_2S-tolerant WGS reactors. Shifted syngas exiting the WGS reactors is made up mostly of H_2 and CO_2, along with some H_2S. A physical solvent (Selexol) is used to absorb in turn H_2S and CO_2 from the syngas in separate units. On depressurization these acid gases are released and recovered as relatively pure streams, and the solvent is regenerated for reuse. If there were no regulations restricting SO_2 or CO_2 emissions, the H_2S would be burned and both SO_2 and CO_2 would be released to the atmosphere. For the first case shown in Table 5 (CO_2 vented) it is assumed that SO_2 emissions are restricted, and that the H_2S is converted to elemental S in a Claus plant, with a SCOT plant provided for tailgas clean-up. The H_2-rich (CO_2- and H_2S-depleted) syngas is then purified using a pressure swing adsorption (PSA) unit, and purge gases recovered from the PSA unit are burned in the combustor of a combined cycle plant to make electricity to meet on-site electricity requirements plus a modest amount of additional electricity that is exported to the electric grid. The effective efficiency[13] for making H_2 from coal in this manner is 63.7 %. If the electricity co-product is valued at the cost of producing electricity in a stand-alone coal IGCC plant with CO_2 vented (see Table 2c), the cost of making H_2 in this manner[14] is $ 6.6/GJ ($ 0.79/kg), if the coal price is $ 1.0/GJ (see Table 5).

Alternatively, the CO_2 could be recovered, dried, compressed (to 150 bar) to make it ready for underground disposal, transported by pipeline to a suitable disposal site, where it would be injected into a suitable underground storage medium via injection wells. Most regions of the world have suitable geologies for such underground storage (see Box 6). Performance and costs are presented in Table 5 for a case where a disposal reservoir is available 2 km underground at a site 100 km from the H_2 production plant. For this CO_2 capture/storage option, which has a CO_2 emission rate that is only 7.5 % of the emission rate with CO_2 vented, the effective efficiency of making H_2 is 60.4 % (5.5 % energy penalty) and the H_2 cost is $ 8.0/GJ (see Table 5) or $ 0.96/kg (21 % cost penalty), and the cost of CO_2 emissions avoided is $ 38/t

of carbon (tC). For comparison, the cost of CO_2 emissions avoided for a decarbonized coal IGCC power plant[15] is $ 86/tC for the same CO_2 disposal arrangement (see Table 2c). Carbon capture and storage is much less costly for H_2 manufacture than for IGCC electricity generation because in the H_2 case the WGS reactors and gas separation equipment are inherent parts of the H_2 manufacturing process even if the CO_2 is vented (all of the incremental capital cost and nearly all of the energy penalty for CO_2 capture in the H_2 case are associated with drying and compressing CO_2), whereas in the IGCC case such equipment is not required if electricity is made and the CO_2 is vented but is required if CO_2 is captured/stored.

Another possibility for avoiding CO_2 emissions is to capture and store H_2S and CO_2 together underground – the co-capture/co-storage option in Table 5. This option, which avoids some costs of capturing these acid gases separately and reducing the H_2S to elemental S, would reduce the H_2 production cost penalty for CO_2 capture/storage to 11 %, and the cost of CO_2 emissions avoided would be only $ 19/tC for the same CO_2 disposal arrangement. The extent to which underground co-storage is a viable option is not yet known, although good operating experience with 39 projects in western Canada[16] that involve co-storage of various mixtures of H_2S and CO_2 in depleted oil and gas fields and in deep aquifers as an acid gas management strategy in conjunction with sour natural gas production is promising and legally permitted [Bachu and Gunter, 2003].

If the H_2 used to make DCL syncrude were decarbonized, the fuel-cycle GHG emission rate relative to petroleum crude-derived gasoline would be reduced from 1.6 to 1.0 if the HTI estimates of energy balances for DCL technology (Table 1a) prove to be valid, or from 1.9 to 1.3 if instead the Bechtel/Amoco estimates (see Table 1b) prove to be valid. The cost of CO_2 capture and storage would increase the synfuel production cost only modestly: by $ 1.2 to $ 1.5 per barrel if co-capture/co-storage of H_2S and CO_2 proves to be a viable acid gas management strategy or $ 2.4 to $ 2.9 per barrel of syncrude if not[17]. But CO_2 capture and storage would not be pursued without a climate change mitigation policy that would value CO_2 emissions at levels of at least $ 20/tC (H_2S/CO_2 co-capture/co-storage case) to $ 40/tC (CO_2 capture/storage case).

2.3.2. ICL technologies

For ICL technologies that produce only a synthetic fuel with CO_2 vented, the fuel-cycle GHG emission rate would be high – about 1.8 times that for the petroleum crude oil-derived products they would replace (see RC-V options in Tables 2a and 2b). As in the case of DCL technologies, however, there are opportunities to reduce GHG emissions via either CO_2 capture/storage or H_2S + CO_2 co-capture/co-storage. But unlike the situation for DCL technologies there are system configurations where H_2S + CO_2 co-capture/co-storage as an acid gas management strategy offers fuel-cycle GHG emission rates significantly lower than for petroleum crude oil-derived fuels, prospectively at synthetic fuel costs that are less than for

system configurations in which the CO_2 is vented! In other words, *there might be significant opportunities for GHG mitigation with some ICL options, even in the absence of an explicit climate change mitigation policy, as an ancillary benefit of an acid gas management strategy involving co-capture/co-storage.*

An appreciation of this counter-intuitive finding requires some understanding of energy and material balances and costs for making fuels via ICL. These processes are briefly described here for MeOH and DME manufacture and in detail in a companion paper [Larson and Ren, 2003].

As in the case of H_2 manufacture, the ICL process for making synthetic carbon-based fuels from coal involves O_2-blown gasification to produce syngas, gas cooling, gas clean-up, WGS, and acid gas (H_2S/CO_2) removal. Subsequently the cleaned syngas is converted catalytically to the desired fuel in a synthesis reactor, followed by separation of unconverted syngas from the liquid fuel product. At this point there are two alternative options. In one plant configuration (the lower "recycle" (RC) option in Figure 1), most of the unconverted gas from the product recovery area is returned to the synthesis reactor to generate additional liquid fuel. The remaining unconverted gas fuels a power cycle making only enough power to meet the process needs. In the other plant configuration (the upper "once-through" (OT) option in Figure 1), syngas passes only once through the synthesis reactor, obviating the need for syngas recycle equipment. The unconverted syngas is used as fuel in a cycle that provides power for export to the grid as well as for on-site power needs.

New slurry-phase synthesis reactor technology makes the OT configurations interesting for CO-rich syngas (such as that generated from coal) by making possible attractive syngas conversion to the synthetic fuel in a single pass [Larson and Ren, 2003]. The OT option offers as one potential attraction significant partial decarbonization opportunities at low incremental cost.

One of the analytic challenges posed by OT technologies producing synthetic fuels and electricity simultaneously is that there is no unique way of allocating GHG emissions between the synfuel and electricity. The approach adopted here is to assign all CO_2 emissions from the plant to the electricity produced, so that the only fuel-cycle GHG emissions associated with the synthetic fuel are upsteam emissions from the synfuel's "share" of the coal consumed plus the CO_2 emissions associated with eventual synfuel combustion[18]. The methodology for calculating fuel-cycle GHG emissions for both OT and RC ICL technologies and the rationale for the emissions allocation scheme chosen for OT systems are discussed in Appendix A.

The partial decarbonization opportunity arises from the prospect that co-capture and co-storage of H_2S and CO_2 as an acid gas management strategy is a potential low-, zero-, or even negative-cost option for reducing CO_2 emission rates. To illustrate the possibilities, the basic ideas involved are elaborated by considering six alternative configurations for making either MeOH or DME:
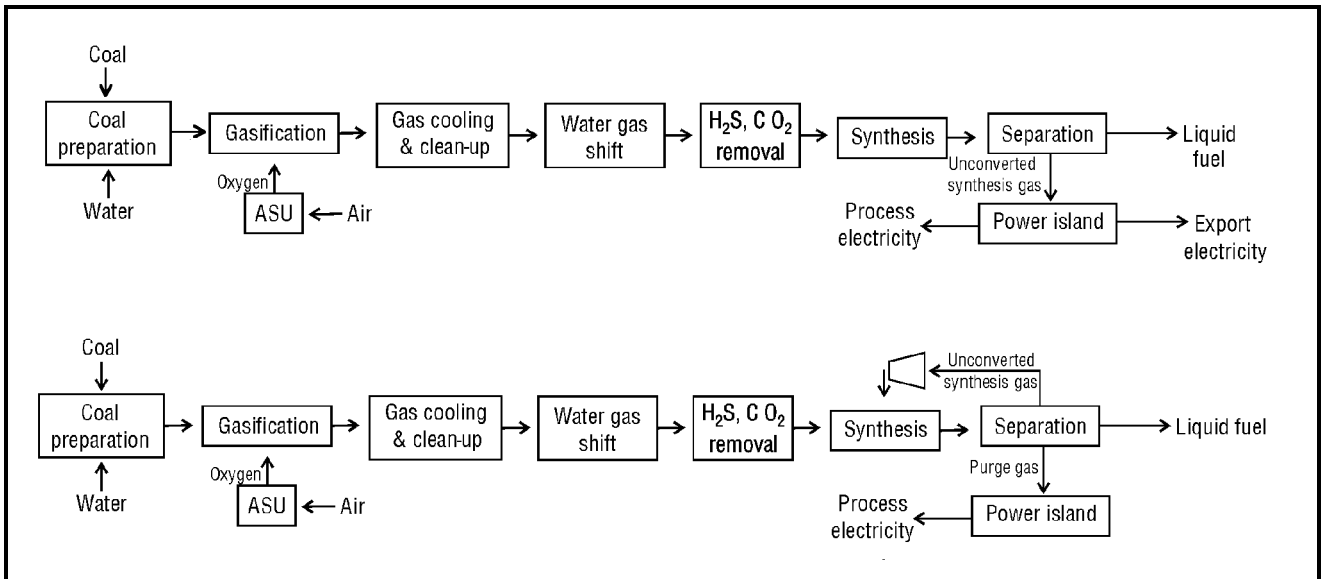
Figure 1. General system layout for making synthetic fuels from coal via ICL

Two alternative system configurations for fluid fuel production from coal via gasification are shown. The configuration at the top represents "once-through" (OT) synthesis with exportable electricity co-product. The configuration at the bottom represents "recycle" (RC) synthesis with no net exportable electricity co-product.
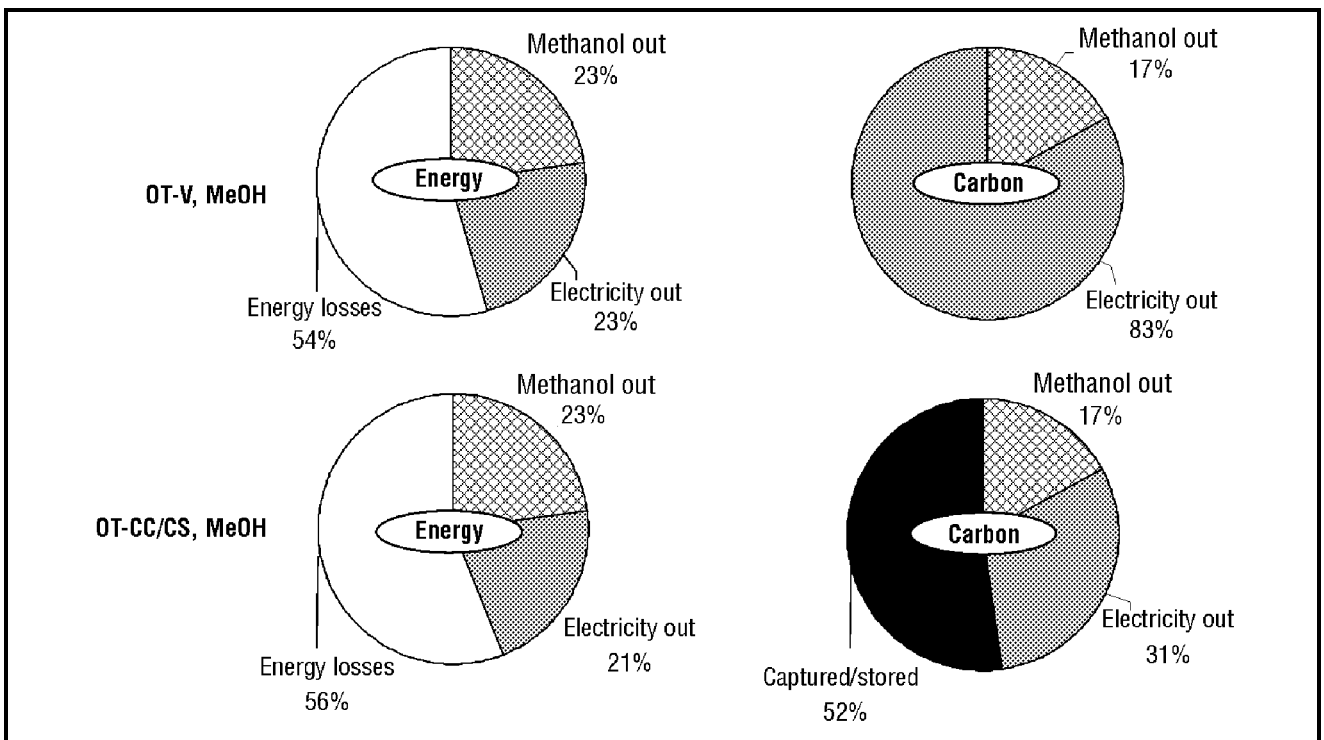

Figure 2. Energy and carbon distributions for MeOH/electricity co-production from coal

three once-through (OT) systems and three recycle (RC) systems – with CO$_2$ vented (V), captured/stored (C/S), and co-captured/co-stored (CC/CS) (see Tables 2a and 2b), with a focus on the CC/CS options. All the MeOH options considered produce 626 MW of MeOH; all the DME options considered produce 600 MW of DME. The energy and carbon balances for the OT-V and OT-CC/CS options are shown in Figure 2 for MeOH and in Figure 3 for DME.

Key to realizing low-cost CO$_2$ capture is the use of WGS reactors upstream of the synthesis reactors. These WGS reactors are not strictly necessary, since some WGS reaction takes place in the synthesis reactor. But without

an upstream WGS reactor, single-pass conversion in the synthesis step is low. Putting in an upstream "partial" WGS reactor to increase the H$_2$/CO ratio to the level that maximizes single-pass conversion ($\sim$ 2 for MeOH and $\sim$ 1 for DME) is often desirable. After exiting the upstream WGS reactor, the shifted syngas is cooled before clean-up.

Because synthesis reactor catalysts are extremely sensitive to various trace contaminants, these must be removed ahead of the synthesis reactor. As noted earlier, most trace metals and other contaminants can be removed at low cost using an activated carbon filter. Subsequently, both H$_2$S and CO$_2$ are removed from the cooled syngas
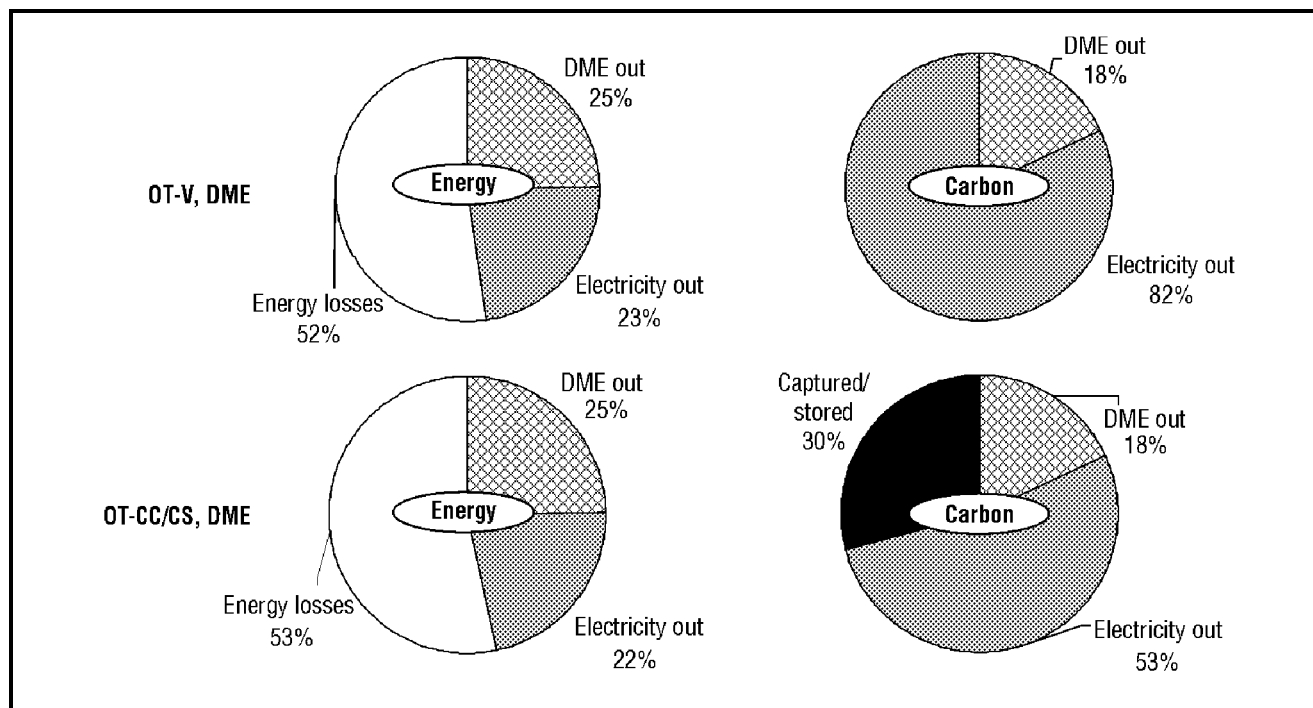
Figure 3. Energy and carbon distributions for DME/electricity co-production from coal

ahead of the synthesis reactor. The syngas must be cleaned of H_2S to ppb levels to protect synthesis reactor catalysts. Much of the CO_2 must be removed to maximize synthetic fuel production[19]. The recovered CO_2 might be vented, but not the highly toxic H_2S. The H_2S might be flared and thereby converted to less toxic SO_2, but air-quality regulations often prohibit such flaring. A typical practice in making chemicals from coal or petroleum residuals has been to recover the H_2S and reduce it to elemental sulfur, which might be sold as a by-product. However, once a large coal gasification-based fuel industry is established, the by-product value of sulfur will be negligible in many cases. An alternative approach that avoids the costs of separating the H_2S from CO_2 and reducing it to elemental sulfur is capture of the acid gases H_2S and CO_2 together for underground storage, as discussed above in the case of making H_2 from coal and as is now common practice as an acid gas management strategy for sour natural gas projects in Canada [Bachu and Gunter, 2003].

Consider the OT-CC/CS cases for both MeOH and DME. In both instances, the fuel-cycle GHG emissions for the synfuels produced are about 0.8 times the rates for the conventional crude oil-derived hydrocarbon fuels they would displace, while the GHG emission rates for the electricity co-products (which are produced at rates comparable to the synfuel production rates) are about 0.5 and 0.8 times the rate for a 33 %-efficient coal steam-electric plant in the MeOH and DME cases, respectively[20]. The greater GHG emission rate reduction realizable in the MeOH case arises because much more upstream shifting is required (to $H_2/CO \sim 2$, compared to $H_2/CO \sim 1$ for DME). However, the cost of avoiding GHG emissions relative to the least-costly CO_2 venting option[21], though low for the MeOH OT-CC/CS case (\$ 18/tC), is lower (actually negative!) for DME (- \$ 15/tC);

the OT-CC/CS configuration actually provides DME at the least cost of the six DME systems considered. The significant avoided cost difference between the MeOH and DME OT-CC/CS cases arises because in both cases the same H_2S processing costs are avoided, but in the MeOH case the CO_2 removal rate/GJ of fuel produced, and thus the cost of CO_2 capture, is almost twice as large.

That the H_2S/CO_2 co-capture/co-storage acid gas management strategy is an option for getting experience with underground storage of CO_2 even before a climate policy is implemented is illustrated by considering that, in some important applications, there are reasonably good prospects that synfuels produced in this manner can be provided at competitive costs. The index chosen to measure a synfuel's competitiveness as an alternative to conventional hydrocarbon fuels is the break-even crude oil price (BCOP, in \$/barrel) defined in Box 8 – an index that neglects environmental and energy supply security benefits.

BCOPs for MeOH and DME are presented for US conditions in Tables 2a and 2b. These BCOPs are \$ 32 to \$ 45 per barrel for MeOH and \$ 37 to \$ 50 per barrel for DME, if advantage is not taken of potential energy efficiency benefits offered by these fuels. However, as discussed above, there are opportunities for using both MeOH and DME more efficiently than hydrocarbon fuels. If it is assumed that MeOH is worth 1.15 times as much as gasoline when used in SIE vehicles because a MeOH engine can be optimized for higher efficiency than a gasoline engine, the BCOP for MeOH falls to about \$ 30 per barrel for the OT-CC/CS option[22]. Moreover, if it is assumed that DME used in CIE cars is worth 1.185 times as much as gasoline used in SIE cars to reflect the inherent efficiency advantage offered by CIE engines compared to SIE engines, the BCOP for DME falls to a very attractive level of about \$ 24 per barrel for the OT-CC/CS case.

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Box 7. The cost of CO₂ disposal

The estimated CO_2 disposal costs C_D (in \$/t of CO_2) for the energy systems described in Tables 2a, 2b, 2c, and 5 are based on a CO_2 disposal cost model developed in Ogden [2002], which calculates for pure streams of CO_2 available at 150 bar,

$C_D = C_{PT} + C_{DW} + C_{SF}$, where:

C_{PT} = cost of pipeline transmission,

C_{DW} = cost of disposal wells, and

C_{SF} = cost of surface facilities near disposal wells, assuming: (1) a 15 % annual capital charge rate (but neglecting interest during construction), (2) an annual O&M cost of 4 % of the capital cost, and (3) an 85 % annual average capacity factor for the system.

The pipe cost $C(Q,L)$ (in \$/m) for pipeline of length L (in km) and CO_2 flow rate Q (in t/day) is given by: $C(Q,L) = (\$700/m) \times (Q/Q_o)^{0.48} \times (L/L_o)^{0.24}$, where Q_o = 16,000 t/day and L_o = 100 km. Thus, C_{PT} = $(0.19/year) \times (1000\ m/km) \times (L\ km) \times C(Q,L)/(Q \times 0.85 \times 365\ days/year)$.

The cost DW (in \$) per disposal well of depth D (in km) is given by

DW = (\$1.25 million/km) × (D km) + \$ 1.0 million. Thus, for N wells,

C_{DW} = $(0.19/year) \times (N \times DW)/(Q \times 0.85 \times 365\ days/year)$. It is assumed that the maximum disposal rate per well is 2500 t/d, so that N = first integer greater than Q/2500.

The cost of surface facilities C_{SF} depends on the detailed layout of pipes and is given by:

C_{SF} = $(0.19/year) \times \$700/m \times \{[(Q/Q_o) \times (L/L_o)^{0.5}]^{0.4}/(N)^{0.5}\}^{1.2} \times (N-1) \times 2 \times (6223m) \times [Q/(N \times 2500)]^{0.5}/[0.85 \times Q \times 365\ days/year]$.

For all cases discussed in this paper, aquifer disposal (see Box 6) is assumed (i.e., no credit is taken for using CO_2 for enhanced resource recovery), with L = 100 km and D = 2 km.

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Since the fuel-cycle GHG emission rate of coal-derived DME is 0.79 times that for gasoline[23], a shift from today's gasoline SIE cars to DME CIE cars would reduce GHG emissions/km to 0.79/1.185 = 0.67 times the rate for gasoline cars[24]. As noted earlier, DME's outstanding air pollutant emission characteristics and quiet operation make it a much stronger candidate than diesel for cars and thus for exploiting the efficiency advantages of CIEs in cars.

2.4. Suitability for the transition to a highly decarbonized energy future

In the longer term, when global climate change considerations will have a powerful influence on energy planning in all countries, it is likely that the major energy carriers will be electricity, H_2, and at least one carbon-based energy carrier provided in such ways that GHG emissions for the global energy system will be about 50 % of those at present or less [TFEST, 2003]. The need for

at least one carbon-based energy carrier in the long term stems from the prospect that H_2 will be used mainly in cities. For rural areas and small towns carbon-based fuels would be needed, because H_2 infrastructure is very costly at low energy-use densities. The use of carbon-based fuels in rural areas and small towns can be consistent with the goal of limiting CO_2 emissions worldwide to half the current level because only a small fraction of society's total energy use will be consumed in such areas. The carbon-based energy carrier or carriers that will be used in the long term should be suitable for use in energy-efficient end-use devices and should generate low levels of air pollutants without complicated exhaust gas after-treatment technology. Can either DCL or ICL technology make it possible to evolve major roles for coal in a world with severe climate and environmental constraints?

DCL technology would not help coal evolve to play major roles in such a long-term energy future. DCL provides only liquid fuels that are not likely ever to be less carbon-intensive and polluting than crude oil-derived fuels, and DCL's poor prospects for making high-quality diesel fuel make it difficult to reduce energy consumption using energy-efficient end-use technologies.

In contrast, near-term deployment of ICL systems in OT configurations would put into place technologies that could evolve over time into systems, such as the one shown in Figure 4, that provide from the same facility a carbon-based fuel plus electricity and H_2, with the latter two energy carriers provided with near-zero CO_2 emissions. The carbon-based fuel could be a fuel such as DME that is versatile, inherently cleaner and less carbon-intensive than today's oil-derived hydrocarbon fuels, and suitable for use in energy-efficient end-use devices. Part of the carbon in the coal might be removed ahead of the synthesis reactor as CO_2 along with H_2S and stored underground as an acid gas management strategy. The unconverted syngas exiting the synthesis reactor could be shifted, generating mainly CO_2 and H_2. This CO_2 could be separated out and stored underground. Some of the H_2-rich syngas could be burned in a combined cycle power plant to make electricity. The rest could be sent to a PSA unit to make pure H_2. The relative amounts of H_2 and electricity produced would depend mainly on relative demands, as there do not seem to be thermodynamic or cost advantages for particular H_2/electricity production ratios [Chiesa et al., 2003; Kreutz et al., 2003]. Thus, before a H_2 economy is established only electricity would be produced as the co-product of the carbon-based synfuel, but the fraction of unconverted syngas converted to H_2 would rise over time as the H_2 economy evolves.

Thus if geological storage of CO_2 proves to be a viable option in widespread applications, ICL technologies would make it possible for coal to play major roles in a climate- and otherwise environmentally-constrained world.

2.5. Supporting technological infrastructures

Introducing any new technology is disruptive of the status quo and institutionally challenging. The challenges are especially daunting during the period of technology scale-up.
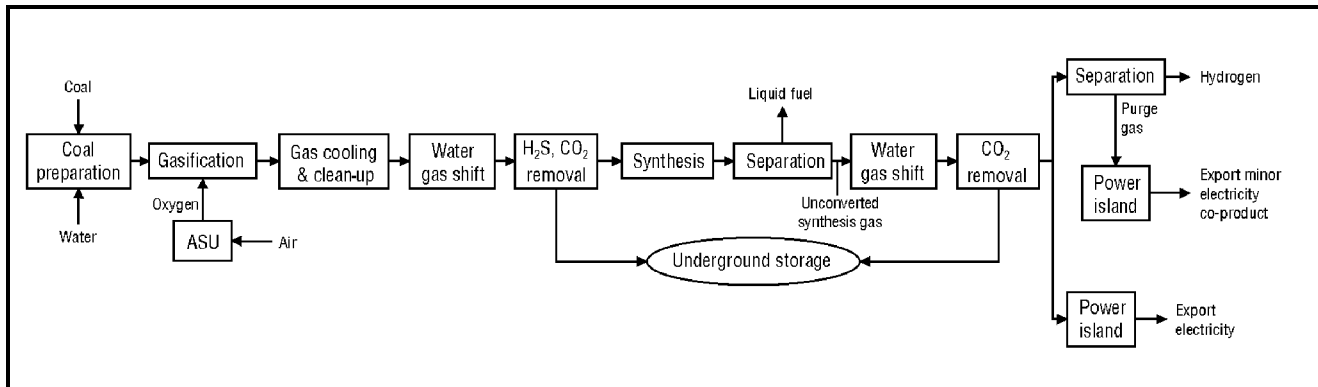
Figure 4. Liquid fuel, electricity and H_2 from coal with low system-wide emissions

This shows how the OT system described in Figure 1 might be modified to include production of H_2 as well as electricity from the syngas that is not converted to liquid fuel in a single pass through the synthesis reactor. In this case both the H_2 and electricity co-products of liquid fuel manufacture would be produced with near-zero CO_2 emissions.

The ease of introducing new synfuel technologies in China depends on the supporting technological infrastructure available, both within China and worldwide.

With the major exception of the H_2 production technology, most DCL system components require new technologies, which make especially daunting the challenges posed in scaling up the technology 1400-fold from the previous largest pilot plant for the first train of the DCL plant that was to be built in Inner Mongolia.

In contrast, for the ICL technologies described above, the only relatively new technological component is the liquid-phase reactor for MeOH and DME synthesis – all other components are well established in chemical process industry markets either in China or elsewhere in the world. The liquid-phase reactor is commercially established for F-T technology and commercially ready for MeOH applications. For the latter, a 10-fold scale-up would be required to produce MeOH at the scale of plants considered in Table 2a relative to what has already been achieved in the successful US DOE-sponsored demonstration project [Heydorn et al., 2003]. Although liquid-phase-reactor technology for DME has not yet been demonstrated at commercial scale, the same reactor already developed for MeOH production can be used for DME, with the addition of an appropriate MeOH dehydration catalyst.

Both DCL and ICL technologies are based on coal chemical process technologies, for which the industrial base is much stronger in China than elsewhere, because China's chemical industry is based mainly on coal as a chemical feedstock. However, the supporting technological infrastructure is much stronger for ICL than for DCL, because China's chemical industry is to a large extent based on syngas derived via gasification. China has extensive experience with syngas and modern coal gasification technology in its chemical industry, where the syngas capacity is about 9 GW (compared to 10 GW in North America) [SFA Pacific, 2000]. This technological base provides a strong foundation for expansion into "polygeneration" – co-production of chemicals, fuels, and electricity

It is also important to consider the supporting technological infrastructure outside China. Industrialized countries have abandoned DCL technologies for making

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Box 8. The break-even crude oil price

When a synthetic fuel is substituted for a conventional hydrocarbon fuel, the break-even crude oil price BCOP (in \$/l) is calculated as BCOP = $(PC_{sf} \times HV_{hcd})/EGF_{sf} - RM_{hcd}$, where:

PC_{sf} = synfuel production cost (in \$/MJ),

HV_{hcd} = volumetric heating value of the conventional hydrocarbon fuel displaced (assumed to be low sulfur gasoline (31.44 MJ/l) or diesel (35.68 MJ/l) – see Table 4),

EGF_{sf} = efficiency gain factor when synfuel displaces the conventional hydrocarbon fuel (both EGF_{sf} = 1.0 cases (no efficiency gain for MeOH displacing gasoline or DME displacing diesel) and cases with EGF_{sf} = 1.15 for MeOH displacing gasoline and EGF_{sf} = 1.185 for DME displacing gasoline are considered), and

RM_{hcd} = refinery margin (\$/l) for the conventional hydrocarbon fuel displaced.

During 1992-2001, when the crude oil price averaged \$ 20.7/barrel, margins at US refineries averaged \$ 0.0716/l for gasoline and \$ 0.0465/l for distillate [EIA, 2002] – all quantities expressed in 2002 US\$. In calculating the BCOP for US conditions, the refinery margin for gasoline is assumed to be equal to the historical average value of \$ 0.0716/l, but the margin for diesel is assumed to be \$ 0.0465 + \$ 0.0132 = \$ 0.0597/l, because it is estimated that compliance with the EPA regulation that diesel sulfur content must not exceed 15 ppm by 2007 will add \$ 0.05/gallon (\$ 0.0132/l) to the cost of diesel [EPA, 2001].

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synthetic fuels for use in their own countries [PCAST, 1997]; interest in synthetic fuels in these countries is focused instead on syngas-based technologies – GTL technologies that can exploit low-cost stranded natural gas supplies and ICL technologies. Both activities can be helpful to China in launching ICL technology in the market. The ongoing rapid growth in gasification markets worldwide is especially relevant for China, with

Table 5. Performances and costs for producing H2 from coal in alternative configurations – US construction[1]

CO$_2$ is:	vented[2]	captured/stored[2]	co-captured/co-stored[2]
H$_2$ output rate (MW)	1070.3	1070.3	1070.3
Coal input rate (MW)	1862.7	1862.7	1862.7
Lifecycle GHG emissions for H$_2$[2] (kg C/GJ H$_2$)	40.00	2.99	1.42
Lifecycle GHG emissions for electricity[2] (g C/kWh)	213.6	213.6	213.6
H$_2$ S removal rate (t H$_2$S/h)	9.79	9.79	9.79
CO$_2$ disposal rate[3] (t CO$_2$/h)	-	553.5	575.7
CO$_2$ disposal cost[4] ($/t CO$_2$)	-	4.52	4.41
Electric power production (+) and use (-) (MW$_e$)			
Gas turbine	+ 78.8	+ 78.8	+ 78.8
Steam turbine	+ 139.5	+ 139.5	+ 139.5
Air separation unit	- 53.92	- 53.92	- 53.92
O$_2$ compressor	- 34.41	- 34.41	- 25.6
CO$_2$ compressor	- 4.28	- 43.10	- 45.59
PSA purge gas compressor	- 11.68	- 11.68	- 11.68
Gasification auxiliaries	- 18.63	- 18.63	- 18.63
Power island auxiliaries	- 2.36	- 2.36	- 2.36
Selexol auxiliaries	- 11.04	- 11.04	- 11.04
Heat rejection	- 3.66	- 4.30	- 14.30
Net power output (MW$_e$)	78.4	38.9	36.4
Effective efficiency of H$_2$ production[5] (%)	63.7	60.4	60.2
Plant capacity factor (%)	85	85	85
Capital cost by component			
Coal storage, preparation, handling	69.9	69.9	69.9
Air separation unit	106.2	106.2	106.2
O$_2$ compressor	5.6	5.6	5.6
CO$_2$ drying and compression	-	41.1	42.7
PSA purge gas compressor	8.8	8.8	8.8
Gasifier and scrubbing	152.8	152.8	152.8
Water gas shift reactors and heat exchangers	61.3	61.3	61.3
Selexol H$_2$S removal and stripping	83.0	83.0	-
Selexol CO$_2$ absorption and stripping	58.5	58.5	-
Selexol for CO$_2$ + H$_2$S capture	-	-	58.5
H$_2$S stripping	-	-	46.6
Sulfur recovery (Claus, SCOT)	56.5	56.5	-
Pressure swing adsorption (PSA)	22.3	22.3	22.3
Gas turbine	30.6	30.6	30.6
HRSG and steam turbine	74.4	74.4	74.4
Power island balance-of-plant + electrics	35.5	35.5	35.5
Total overnight construction cost ($10^6)	765.4	806.5	715.5
Interest during construction[6] ($10^6)	122.7	129.2	114.5
Total capital cost ($10^6)	888.1	935.8	830.0
Specific overnight construction cost ($/kW H$_2$)	715	753	669

Table 5 (contd.). Performances and costs for producing H_2 from coal in alternative configurations – US construction[1]

CO_2 is:	vented[2]	captured/stored[2]	co-captured/co-stored[2]
H_2 production cost[6] ($/GJ)			
Capital	4.64	4.89	4.34
Operation and maintenance	1.07	1.12	1.00
Coal input (for coal @ $1.0/GJ)	1.74	1.74	1.74
Electricity credit[7] (P_E = electricity price in $/kWh)	$-20.35 \times P_E$	$-10.10 \times P_E$	$-9.45 \times P_E$
CO_2 disposal[4]	-	0.65	0.66
Total	$7.45 - 20.35 \times P_E$	$8.40 - 10.10 \times P_E$	$7.74 - 9.45 \times P_E$
Total for P_E = $ 0.0429/kWh[8]	6.58	7.97	7.33
Cost of GHG emissions avoided[9] ($/t C)	-	38	19

Notes

1. From Chiesa et al. [2003] and Kreutz et al. [2003], with energy balances and material flows calculated for the Texaco O_2-blown gasifier with quench (@ 70 bar) and high-sulfur coal (Illinois No. 6 coal with 24.826 MJ/kg, 3.41 % S, 12.0 % moisture, and a carbon content of 24.68 kg C/GJ).

2. Total fuel-cycle emissions are those for the conversion plant with the assumed coal plus estimated GHG emissions upstream of the plant. It is assumed that 0.8 % of the C in the coal is unconverted and is disposed of with the coal ash. The GHG emissions upstream of the conversion plant are estimated (for typical US conditions) to be 1.0 kgC of CO_2 equivalent (see Note 12 to main text). The specific GHG emissions/GJ of H_2 = (total fuel-cycle emissions/GJ of H_2) - (fuel-cycle emissions/GJ of H_2 for electricity co-product @ 213.6 gC/kWh). The specific GHG emissions allocated to electricity are those for a 390.1 MW_e 43.0 %-efficient stand-alone IGCC plant with CO2 vented – see Table 2c. (The emission rate indicated in Table 2c for an IGCC plant is slightly higher (219.1 gC/kWh) because the assumed coal in that case is Yanzhou bituminous coal rather than Illinois No. 6 coal.)

3. In Chiesa et al. [2003], 91.28 % of the carbon in the coal is recovered as CO_2.

4. The CO_2 disposal cost (in $/t CO_2) is estimated according to the procedure described in Box 7.

5. See Note 13 (to main text).

6. Calculated according to the methodology outlined in Box 5.

7. Electricity is co-produced at a rate of 20.35/10.10/9.45 kWh/GJ H_2 for CO_2 venting/capture/co-capture case.

8. Electricity value = production cost for 390 MW_e coal IGCC plant with CO_2 venting (see Table 2c).

9. Cost of CO_2 emissions avoided for a CO_2 capture option = $(C_{HC} - C_{HV})/(E_{HV} - E_{HC})$, where C_{HC} = H_2 cost ($/GJ) for CO_2 capture option, C_{HV} = H_2 cost ($/GJ) with CO_2 vented, E_{HC}= GHG emissions (tC of CO_2 equivalent/GJ of H_2) for capture option, and E_{HV} = GHG emissions (tC of CO_2 equivalent/GJ of H_2) for CO_2 venting option.

gasification capacity being added worldwide at a rate of 3 GW/year and expected to reach 61 GW by 2004 [SFA Pacific, 2000]. There is also a solid and rapidly growing worldwide technological infrastructure for polygeneration in the petroleum refining industry – mostly based on gasification of petroleum residuals – that can be helpful to China in moving ahead with polygeneration.

3. Prospective ICL synfuel costs in China

Because DCL technologies are so far from being commercially ready, no attempt was made to estimate production costs for DCL-derived fuels in the previous section, but cost estimates were made for coal-derived MeOH and DME (Tables 2a and 2b) (as well as for coal IGCC electricity (see Table 2c)), for plants that might be built in the United States. Here preliminary estimates are made of costs in China for coal-derived MeOH and DME for selected plant configurations (the RC-V and OT-CC/SC options) and for two alternative coal prices ($ 1.0/GJ for a "city-gate" plant and $ 0.5/GJ for a "mine-mouth" plant).

The major challenge in translating the costs in Tables 2a and 2b into costs for China is to estimate how construction costs would differ from US construction costs. Although actual ICL construction costs for China cannot be known for sure until the first ICL plants are actually

built there, there is strong evidence that costs would be less in China, largely because of lower labor costs. The substantial worldwide experience with gasification technologies has led to the development of "location factors" that make it possible to translate cost experience in one region to another with some confidence. This experience suggests that: (1) for both IGCC technology and for the power-generating part of ICL OT plants the capital cost with Chinese construction would be 1/3 less than for US construction[25], and (2) for the synfuel part of ICL plants, the capital cost in China would be 1/4 less than in the US[26]. Under these assumptions estimated costs for making MeOH and DME in China are presented in Table 6, along with comparisons to costs in the United States and to 2002 prices in China for conventional crude oil-derived hydrocarbon fuels that MeOH and DME would be competing with, and BCOPs[27] in China. The estimated MeOH and DME costs with Chinese construction for the least costly configurations shown in Table 6 are close to prices at which several enterprises in China have indicated they would be willing to produce these fuels: about 1000 RMB/t for MeOH and 1400 RMB/t for DME [Ni, 2003]. Notably the Table 6 calculations suggest that: (1) MeOH and DME costs would be as low as or lower than Chinese wholesale hydrocarbon fuel prices in 2002; and (2) the BCOPs for the OT-CC/CS options with energy efficiency

Table 6. Estimated costs and values for MeOH and DME produced in recycle and once-through configurations – for both US and China construction

	MeOH (626 MW or 843,200 t/y)				DME (600 MW or 563,900 t/y)			
Plant configuration[1]	**RC-V**		**OT-CC/CS** (+ 577 MW$_e$ electricity)		**RC-V**		**OT-CC/CS** (+ 526 MW$_e$ electricity)	
Assumed coal price	City gate ($1.0/GJ (243 RMB/tce))	Mine mouth ($0.5/GJ (122 RMB/tce))	City gate ($1.0/GJ (243 RMB/tce))	Mine mouth ($0.5/GJ (122 RMB/tce))	City gate ($1.0/GJ (243 RMB/tce))	Mine mouth ($0.5/GJ (122 RMB/tce))	City gate ($1.0/GJ (243 RMB/tce))	Mine mouth ($0.5/GJ (122 RMB/tce))
Costs based on US construction								
Fuel cost, US$/GJ	8.63[2]	7.78[3]	9.42[2]	8.30[3]	9.50[2]	8.59[3]	8.28[2]	7.29[3]
Fuel cost, US$/t[4]	172	155	187	165	271	245	236	208
Electricity value, US¢/kWh	4.29[5]	3.87[3]	4.29[5]	3.87[3]	4.29[5]	3.87[3]	4.29[5]	3.87[3]
Break-even crude oil price, US$/barrel (if refinery margin = US¢ 7.16/l for gasoline; US¢ 5.97/l for diesel)[6]								
Neglecting efficiency benefit[7]	31.8	27.5	35.7	30.1	44.4	39.2	37.5	31.9
With efficiency benefit[8]	26.1	22.4	29.6	24.7	28.7	24.9	23.5	19.4
Costs based on China construction (if capital cost in China = 0.75 × US cost for fuel-related investment; = 0.664 × US cost for electric power-related investment)[9]								
Fuel cost, US$/GJ	6.91	6.05	7.56	6.44	7.58	6.67	6.65	5.66
Fuel cost, US$/t[4] (RMB/t)[10]	138 (1141)	120 (999)	150 (1249)	128 (1064)	216 (1793)	190 (1578)	190 (1573)	161 (1339)
Electricity value, US¢/kWh (RMB¢/kWh)[10]	3.14[5] (26.1)	2.72 (22.6)	3.14[5] (26.1)	2.72 (22.6)	3.14[5] (26.1)	2.72 (22.6)	3.14[5] (26.1)	2.72 (22.6)
Break-even crude oil price, US$/barrel (if refinery margin = 0.75×7.16 = US¢ 5.37/l for gasoline; 0.75×5.97 = US¢ 4.48/l for diesel)[11]								
Neglecting efficiency benefit[7]	26.0	21.7	29.3	23.7	35.9	30.7	30.6	25.0
With efficiency benefit[8]	21.5	17.8	24.3	19.5	23.4	19.6	19.5	15.3
LPG-equivalent cost, RMB/t[10,4]	-	-	-	-	2890	2550	2540	2170
LPG import price, RMB/t[12]	-	-	-	-	Range of average monthly prices, 2002: 1760 to 2840 (average price for 2002 = 2117)			
Diesel-equivalent cost, RMB/t[10,4]	-	-	-	-	2620	2310	2300	1960
Wholesale diesel price, RMB/t[12]	-	-	-	-	Range of average monthly prices, 2002: 2300 to 3200			
Gasoline-equivalent cost, RMB/t[10,4]								
Neglecting efficiency benefit[7]	2440	2140	2670	2280	-	-	-	-
With efficiency benefit[8]	2120	1860	2320	1980	2260	1990	1980	1690
Wholesale gasoline price, RMB/t[12]	Range of average monthly prices, 2002: 2400 to 3600							

Notes

1. The RV-V and OT-CC/CS are, respectively, from Table 2a for MeOH and Table 2b for DME. Here V = CO_2 vented (recovered H_2S is converted to elemental sulfur; recovered CO_2 is vented); CC/CS = CO_2 co-captured/co-stored (H_2S and CO_2 are recovered together, dried, compressed to 150 bar for transport to disposal site for underground storage).

2. From Table 2a for MeOH and Table 2b for DME.

3. When the coal price is reduced, $1.0 to $0.5/GJ, the electricity value (IGCC electricity cost) is reduced, 4.29 ¢/kWh to 3.87 ¢/kWh -- see Table 2c.

4. Assuming energy values (in GJ/t) of 19.9 for MeOH, 28.5 GJ for DME, 46.0 for LPG, 42.6 for gasoline, and 41.7 for diesel -- see Table 4.

5. See Table 2c.

6. See Box 8.

7. Assuming 1 GJ MeOH is worth 1 GJ gasoline and 1 GJ DME is worth 1 GJ diesel.

8. Assuming 1 GJ MeOH is worth 1.15 GJ gasoline and 1 GJ DME is worth 1.185 GJ gasoline.

9. See Notes 25 and 26 (to main text).

10. Assuming 1 US$ = 8.3 RMB.

11. Assuming that for new refineries in China the margins for refining gasoline and diesel are 0.75 times as large as the US average, 1992-2001.

12. [Yung, 2003].

benefits taken into account would be attractive – $ 24 and $ 20 per barrel at city-gate plants for MeOH and DME, respectively, and BCOPs that are $ 4 to $ 5 per barrel less for mine-mouth plants. Also, a shift from crude oil-derived products to coal-derived ICL products would bring stability to fuel prices; the volatility of the world oil price led in 2002 to monthly average wholesale hydrocarbon fuel prices in China for which peak monthly prices were 1.4 to 1.6 times the least monthly prices (see Table 6).

4. Ascertaining CO_2/H_2S co-capture/co-storage viability for acid gas management

A major finding of this study is that if CO_2/H_2S co-capture/co-storage is viable as an acid gas management strategy, there are some ICL systems for which GHG emissions could be significantly less than for conventional crude oil-derived hydrocarbon fuels, even in the absence of a climate mitigation policy that puts a market price on CO_2 emissions.

However, despite the promising Canadian experience with this acid gas management strategy in conjunction with sour natural gas projects, that experience is not enough to give confidence that this strategy is viable for a wide range of geological media and for large-scale projects – e.g., for the DME OT-CC/CS plant described in Table 2b, the annual CO_2 storage rate is 1.8 Mt/year, whereas the total CO_2 storage rate for all 39 Canadian projects is only 0.25 Mt/year [Bachu and Gunter, 2003]. It is desirable to find out as soon as possible if underground co-storage of CO_2 and H_2S is a viable strategy for widespread applications – as a key part of a broader effort to augment experience to date (see Box 6) and ascertain the viability of underground storage of CO_2 as a major climate change mitigation strategy. Many "mega-scale" (e.g., involving geological CO_2 storage rates ~ 1 Mt of CO_2/year or more) demonstration projects along with appropriate monitoring, modeling, and scientific experiments, in alternative geological contexts, are needed [Williams, 2003].

To keep demonstration project costs low, countries might work together, pooling scarce resources and seeking demonstration sites where CO_2 costs are very low near scientifically interesting prospective CO_2 storage sites. It is very likely that China has some of the least-costly CO_2 sources in the world at its many plants that make ammonia for fertilizer from coal and co-produce streams of relatively pure CO_2. At these plants about half of the CO_2 is typically used to make urea, but the other half is vented. It would be worthwhile to explore whether there are interesting prospective demonstration sites near one or more of these plants and see if other countries might work with China in exploiting demonstration opportunities. It would be particularly desirable to demonstrate in China $CO_2 + H_2S$ co-storage to see if this is a viable sulfur management option for ICL technology in China.

5. Conclusion

This study has compared ICL and DCL technologies for synthetic fuel production from coal and has shown that:

1. ICL technologies would be about as energy-efficient as DCL technologies if end-use as well as production-conversion efficiencies are taken into account;
2. there are ICL-derived fuels such as DME that would outperform both DCL-derived fuels and conventional hydrocarbon fuels in terms of air-quality impacts;
3. ICL technologies offer better GHG emission mitigation prospects than DCL technologies, even in the near term, in the absence of an explicit climate change mitigation policy;
4. deployment now of ICL technologies could put the coal energy system on a track consistent with meeting severe climate and other environmental constraints without having to abandon coal, but deploying DCL technologies could not; and
5. there are much stronger supporting technological infrastructures both within China and worldwide for ICL technologies than for DCL technologies.

Although the study did not assess prospective costs for DCL synfuels because the modest experience with the technology provides an inadequate basis for making meaningful cost projections at this time, cost estimates for ICL-based MeOH and DME technologies based on a companion study [Larson and Ren, 2003] were presented and extended to provide estimates of ICL synfuel costs in China. Especially promising is the outlook for DME produced in once-through configurations: DME is a clean and versatile fuel that would be competitive at present LPG import prices; DME would be able to compete with diesel at crude oil prices of $ 25-31/barrel, and with gasoline in automotive applications at crude oil prices of $ 15-20/barrel; and unlike oil prices, the price of coal-derived DME would not be volatile. Although these cost estimates are also uncertain pending construction experience with actual ICL plants in China, one can have reasonable confidence that these cost estimates are not too far from what might be expected in the real world because of the extensive market experience with most of the technological components involved in these systems, both in China and elsewhere in the world, in chemical and petroleum-refining industry applications.

An important finding is the potential for realizing in the case of DME significant reductions in GHG emissions relative to crude oil-derived hydrocarbon fuels even in the absence of an explicit climate change mitigation policy when DME is produced in once-through plants that co-produce electricity at a rate comparable to the DME production rate. But this finding depends on the viability of H_2S/CO_2 co-capture/co-storage as an acid gas management strategy. "Megascale" demonstration projects along with appropriate monitoring, modeling, and scientific experiments, in alternative geological contexts, are needed worldwide. It is very likely that China has some of the least-costly CO_2 sources in the world for possible use in such demonstrations. It would be worthwhile to explore whether there are interesting prospective demonstration sites near one or more of these sources and see if other countries might work with China in exploiting demonstration opportunities at such sites.

Articles

As a final note, the attractions of ICL-based co-production could potentially hasten a transition to gasification for power generation (compared to gasification for stand-alone IGCC power plants), making possible much earlier exploitation of the many air-pollutant and GHG emission mitigation benefits offered by gasification energy strategies, and lead to a fundamental reorganization of the coal energy industry that would integrate presently separate and uncoordinated activities (power generation and fuel production), with attendant economies of scope, only some of which have been explored in this study. ∎

Notes

1. The lower heating value (LHV) of Yanzhou bituminous coal is 31.71 MJ/kg, moisture and ash-free (MAF) basis.

2. The optimized plant would convert 52.4 % of the coal input energy to useful products: 12,377 barrels per day (b/d) of F-T liquids (28.1 % of coal input energy) plus 676 MW$_e$ of electricity (24.3 % of coal input energy).

3. DME degrades quickly in the troposphere.

4. Energy values in this paper are on a LHV basis unless explicitly indicated otherwise. Only the calculations in Tables 1a and 1b are presented on a HHV basis (as in the original publications). The 75 % and 59 % HHV efficiencies presented in Tables 1a and 1b correspond to LHV efficiencies of 73 % and 58 %, respectively.

5. Assessing the reasons for these very different estimates is beyond the scope of the present study.

6. But, if gasoline were made from MeOH via the Mobil process, additional refining energy would be required.

7. Cyclic hydrocarbon compounds that contain at least one benzene ring, with alternate single and double C-C bonds.

8. This is obtained by solving for α (the DCL refinery energy loss) the equation setting system efficiencies equal for ICL and DCL technologies: $1.15 \times 58.3 = 73 \times (1 - \alpha)$.

9. Particle emissions are not zero despite absence of C-C bonds and near-zero sulfur content, because apparently some particles are generated from the engine's lubricating oil [Fleisch and Meurer, 1995].

10. This is in contrast to the situation for coal steam-electric plants, for which Hg removal costs could be substantial. Consider that in the US, where in 1999 the average Hg emission rate for coal power plants was 2.15×10^{-5} g/kWh, the cost for removing Hg from flue gases of coal steam-electric plants via carbon filters has been estimated to be ~ $ 190/g [EIA, 2001]. Thus, removal of 75 % of the Hg would contribute about $ 0.003/kWh to the cost of generating coal steam electricity -- equivalent to ~ 15 % of the typical short-run marginal generating cost or about $ 5.5 billion per year for the nation as a whole, if Hg controls were required for all 1830 TWh/yr of US coal electricity generation. If instead old steam-electric plants were retired in favor of new coal IGCC plants and Hg control was mandated, the Hg could be recovered via carbon filters at much higher partial pressure from syngas; the cost of removing Hg from the syngas at a 99 % recovery rate has been estimated to be about $ 3/g [Klett and Rutkowski, 2001], so that the incremental cost/kWh at a 99 % recovery rate would be less than 2 % of the incremental cost/kWh calculated above for 75 % recovery at coal steam-electric plants.

11. The fuel-cycle emission rates for gasoline and diesel are, respectively, 1.30 and 1.25 times direct CO_2 emission rates from burning these fuels, based on the Argonne National Laboratory's GREET model (see Table 4).

12. In the Argonne National Laboratory's GREET model, the CO_2-equivalent of upstream GHG emissions for large energy conversion plants under typical US conditions are: (1) for natural gas: 2.84 kgC/GJ (or 2.56 kg C/GJ, HHV) (61.84 % CO_2, 37.66 % CH_4, 0.49 % N_2O); (2) for coal: 1.0 kgC/GJ (or 0.96 kgC/GJ, HHV) (64.6 % CH_4, 35.2 % CO_2, and 0.2 % N_2O). See [Ogden et al., 2004].

13. For a plant making both synthetic fuel and electricity from coal, the effective efficiency η_{eff} for making synfuel is defined as $\eta_{eff} = F_{sf}/(1 - F_e/\eta_e)$, where F_{sf} (F_e) is the synfuel (electricity) output as a fraction of the coal input and η_e is the efficiency of a stand-alone coal IGCC power plant with CO_2 vented ($\eta_e = 0.43$ -- see Table 2c).

14. For US construction. The methodology for energy cost estimates presented in this paper is summarized in Box 5.

15. Decarbonizing coal IGCC plants is far less costly than decarbonizing coal steam-electric plants [Williams, 2003].

16. Canadian acid gas disposal projects began in 1989; since then the number of projects has grown rapidly: to 6 by 1995, 22 by 1998, 31 by 2000, and 39 at the time of this writing.

17. Although no attempt is made in this paper to provide an independent assessment of costs for making synthetic fuels via DCL, one HTI analysis [Comolli et al., 1996] estimates that 1 barrel of syncrude is worth 1.19 barrels of petroleum crude oil (because the syncrude is partially refined), and another HTI analysis [Zhou and Lee, 2003] projects that its DCL technology would be competitive at petroleum crude oil prices above $ 22-$ 28 per barrel. If that projected cost could be realized, there would be no more than about a 10 % cost penalty for the DCL product associated with decarbonizing the needed H_2.

18. Thus the GHG emission rate GER_{sf} (in kgC of CO_2 equivalent/GJ of synfuel) is given by $GER_{sf} = (UGER_c/\eta_{eff}) + C_{sf}$, where $UGER_c$ is the upstream GHG emission rate for coal, C_{sf} is the CO_2 emission rate (in kgC/GJ) from synfuel combustion, and η_{eff} is the effective efficiency of synfuel production (see Note 13).

19. But a small amount of CO_2 must be left in the syngas to ensure good catalyst activity in the synthesis reactor.

20. Alternatively, the GHG emission rates for electricity are 0.65 and 1.02 times the emission rate for a coal IGCC plants with CO_2 vented (from Table 2c) for the MeOH and DME OT-CC/CS cases, respectively.

21. RC-V for MeOH and OT-V for DME.

22. This BCOP is for zero value of CO_2 emissions, so that the electricity co-product is worth the same as for a coal IGCC plant with CO_2 vented ($ 0.043/kWh), even though the GHG emission rate for electricity is 35 % less (see Note 20). If the electricity were instead sold for $ 0.046/kWh, the MeOH cost would fall to the level for the RC-V plant and the BCOP for MeOH would fall to $ 26 per barrel (see Table 2a). At the $ 66/tC avoided cost rate for a coal IGCC plant with H_2S/CO_2 co-capture/co-storage (see Table 2c), reducing IGCC emissions 35 % would instead increase the electricity cost to $ 0.048/kWh -- highlighting the cost advantages of decarbonizing electricity via co-production with a synfuel relative to stand-alone power generation.

23. The fuel-cycle GHG emission rate for DME (OT-CC/CS option) is 20.3 kgC of CO_2-equivalent/GJ (see Table 2b), compared to 26.6 kgC/GJ for gasoline (see Table 4).

24. The GHG mitigation benefits (as well as the energy supply security benefits) of shifting cars from gasoline derived from imported oil to coal-derived DME could be enhanced by improving the end-use efficiency as well as the engine efficiency -- by reducing rolling resistance and aerodynamic drag, by using lighter weight materials, and by shifting to CIE hybrid-electric technology. Weiss et al. [2003]) show that CIE hybrid-electric cars in 2020 could be 2.7 times as energy-efficient as 2001 gasoline SIE cars with the same performance and amenities. For these cars the GHG emission rate per km would be 0.79/2.7 = 0.3 times that for today's gasoline cars.

25. China currently has the capacity to produce all components of IGCC plants except the gas turbine, and experience indicates lower construction costs in China. Shell gasifiers are estimated to cost 0.6 times as much for Chinese as for US construction [Wang, 2002], and General Electric analysts have estimated that coal IGCC plants constructed in China would cost 0.65 times as much as US-constructed IGCC plants [Stoll and Todd, 1996]. If it is assumed that for IGCC plants built in China, the capital cost for each component except the gas turbine is 0.6 times that for a US-built IGCC plant whereas for the gas turbine the capital cost is the same as for a US-built plant, the overall capital cost of an IGCC plant built in China would be 0.664 times the capital cost for a US-built plant.

26. For US construction, the net capital required for fuel production = OCC - (capital for net power generating capacity @ $ 1202/kW (cost for 43 %-efficient coal IGCC plant -- see Table 2c)), where OCC = total overnight construction cost for the entire plant. For China construction, it is assumed that the capital cost for fuel production is 0.75 times the value for US construction -- the China location factor estimated in Lucas [2002] for the proposed Ningxia plant for making DME from coal. The capital cost for the net export power generating capacity with China construction is assumed to be 0.664 times the cost with US construction (see Note 25).

27. In calculating break-even crude oil prices (BCOPs), it is assumed that Chinese refinery margins would be 0.75 times the margins estimated in Box 8 for the United States.

28. Octane is a measure of the tendency of an air/fuel mixture to resist combustion as it is heated during the compression stroke in a cylinder of an ICE engine. The tendency to pre-ignition or "knock" decreases engine efficiency and increases engine wear. In the United States the octane rating is often reported as (RON + MON)/2, where RON = research octane number; MON = motor octane number. This index has the value 99 for MeOH and ~ 88 for a typical gasoline.

29. Typically mixtures of 85-90 % MeOH with 15-10 % gasoline (M85 or M90) are preferred over pure MeOH for automotive use. The addition of gasoline increases the vapor pressure of the fuel enough to facilitate cold starting.

30. At atmospheric pressure DME boils at -24.9°C, so it must be stored in moderately pressurized tanks, as is the case for LPG. For comparison, propane boils at -42.1°C and butane at -0.5°C.

31. Both DME and MeOH are relatively easy to reform because they have no carbon-carbon

bonds to break; but the first step in reforming MeOH is to apply heat to vaporize it -- a step that is not needed for DME, a gas at atmospheric pressure.

32. The critical point for CO_2 is 74 bar and 31ºC.

33. Because the hydrostatic pressure gradient is typically about 100 bar/km.

34. Deep aquifers (~ 800 m or more below the surface) tend to be saline because the contained water is fossil water that has been there over geological time -- time sufficient for the water to come into chemical equilibrium with the minerals in the host rock. Dissolved salts typically make the water brackish and often even briny.

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Appendix A. GHG emissions and costs of GHG emissions avoided for ICL technologies

Here is the methodology for calculating fuel-cycle GHG emissions and costs for GHG emissions avoided for ICL technologies is developed – first for recycle (RC) plants and then for once-through (OT) plants that produce electricity as well as a synthetic fuel.

A1. GHG emssions and costs of emissions avoided for recycle plants

For RC synthetic fuel-producing plants calculations are presented in turn for fuel-cycle-wide GHG emissions and costs of avoiding emissions.

A1.1. Fuel-cycle GHG emissions

The fuel-cycle GHG emission rate GER_{sf} (in kgC of CO_2 equivalent/GJ of synfuel) is made up of direct CO_2 emissions PER_{sf} from the production process, plus emissions C_{sf} when the synfuel is burnt or its carbon content is otherwise released to the atmosphere, plus upstream GHG emissions $UGER_{sf}$ involved in coal-mining and transport to the conversion plant, plus downstream emissions DER_{sf} that arise between its production and ultimate consumption. Here DER_{sf} is assumed to be negligible, so that fuel-cycle emissions are approximated as:

$GER_{sf} = PER_{sf} + UGER_{sf} + C_{sf}$, where

$PER_{sf} = (C_c/\eta_{eff}) - C_{sf} - CSR_{sf}$,

$UGER_{sf} = UGER_c/\eta_{eff}$,

$UGER_c$ = upstream GHG emission rate for coal consumed at plant (= 1.0 kgC/GJ (see Note 12)).

C_c = carbon content of coal input (= 25.17 kgC/GJ),

C_{sf} = carbon content of the synfuel,

CSR_{sf} = rate of storing CO_2 underground for synfuel manufacture (kgC/GJ of synfuel).

$\eta_{eff} = F_{sf}/(1 - F_e/\eta_e)$ = effective efficiency (allocates to synfuel only coal consumed above that needed to produce the same amount of power in stand-alone coal IGCC plant with CO_2 vented),

η_e = efficiency of a stand-alone coal IGCC plant with CO_2 vented (= 0.43),

F_{sf} = synfuel energy output as fraction of coal energy input rate,

F_e = electricity output as fraction of coal energy input rate (negative for import cases), so that:

$GER_{sf} = [(C_c + UGER_c)/F_{sf}] \times (1 - F_e/\eta_e) - CSR_{sf}$.

A1.2. Cost of GHG emissions avoided

The cost of GHG emissions avoided C_{ea} (in \$/tC) for an RC option with CO_2 capture is:

$C_{ea} = (CST_{sf\ RC-C} - CST_{sf\ LC-V})/(GER_{sf\ RC-V} - GER_{sf\ RC-C})$, where:

$CST_{sf\ RC-C}$ = synfuel cost (\$/GJ) for RC capture (C) option,

$CST_{sf\ LC-V}$ = synfuel cost (\$/GJ) for the least-costly synfuel venting (V) option,

$GER_{sf\ RC-C}$ = GHG emissions (tC CO_2 equivalent/GJ) for C option, and

$GER_{sf\ LC-V}$ = GHG emissions (tC CO_2 equivalent/GJ of synfuel) for least-costly V option.

A2. GHG emissions and costs of emissions avoided for once-through plants

There is no unique way of allocating GHG emissions between the fuel and electricity co-products for OT options. The approach adopted is responsive to the need in a climate-constrained world to measure emissions relative to the limits of what is achievable in principle (without violating physical or chemical laws).

A2.1. Fuel-cycle GHG emissions

Because fuel-cycle-wide GHG emissions associated with a synfuel cannot be less than the CO_2 generated when the synfuel is burned or its C content is otherwise released to the atmosphere, whereas emissions from making electricity can in principle be reduced to zero via CO_2 capture and storage, all direct CO_2 emissions associated with synfuel manufacture are allocated to electricity. Thus direct CO_2 emissions allocated to the synfuel are $PER_{sf} = 0$, and emissions PER_e (in gC/kWh) allocated to the electricity co-product are:

$$PER_e = (1000 \text{ g/kg}) \times (C_c/F_{sf} - C_{sf} - CSR_{sf})/ECR_{sf}, \text{ where:}$$

ECR_{sf} = electricity co-production rate (kWh/GJ of synfuel). Fuel-cycle GHG emissions are made up of these PER rates plus emissions in end-use (C_{sf} for the synthetic fuel but $C_e = 0$ for electricity), plus upstream GHG emissions $UGER_{sf}$ and $UGER_e$ arising from coal-mining and transport to the conversion plant, plus downstream emissions DER_{sf} and DER_e that arise between production and ultimate consumption (both of which are neglected), so that fuel-cycle emissions are approximated as:

$GER_{sf} = UGER_{sf} + C_{sf}$ (in kgC of CO_2 equivalent/GJ) for synfuel, and

$GER_e = UGER_e + PER_e$ (in gC of CO_2 equivalent/kWh) for electricity, where:

$UGER_{sf} = UGER_c/\eta_{eff} = (UGER_c/F_{sf}) \times (1 - F_e/\eta_e)$, and

$UGER_e = (1000 \text{ g/kg}) \times UGER_c \times [(0.0036 \text{ GJ/kWh})/\eta_e]$, so that:

$GER_{sf} = (UGER_c/F_{sf}) \times (1 - F_e/\eta_e) + C_{sf}$, and

$GER_e = (1000 \text{ g/kg}) \times \{[GER_c/F_{sf} - C_{sf} - CSR_{sf}]/ECR_{sf} + UGER_c \times [(0.0036 \text{ GJ/kWh})/\eta_e]\}$.

A2.2. Cost of GHG emissions avoided

The cost of GHG emissions avoided C_{ea} (in \$/tC) for an OT option with CO_2 capture is:

$$C_{ea} = (CST_{sf/e \text{ OT-C}} - CST_{sf/e \text{ LC-V}})/(GER_{sf/e \text{ LC-V}} - GER_{sf/e \text{ OT-C}}),$$

where:

$CST_{sf/e \text{ OT-C}}$ = Cost for the OT C option of synfuel + electricity (\$/GJ of synfuel),

$CST_{sf/e \text{ LC-V}}$ = Cost for the least costly V option for synfuel + additional IGCC electricity such that total electricity is the same as for OT-C option (\$/GJ of synfuel),

$GER_{sf/e \text{ OT-C}}$ = GHG emissions (tC of CO_2 equivalent/GJ synfuel) for C option, and

$GER_{sf/e \text{ LC-V}}$ = GHG emissions (tC of CO_2 equivalent/GJ synfuel) for least-costly V option + additional IGCC electricity such that total electricity is the same as for OT-C option.

Readers' reactions welcomed

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"Correspondence"
C/o the Editorial and Production Coordinator
Energy for Sustainable Development
25/5, Borebank Road
Benson Town
Bangalore-560 046
India
Fax: +91 80 353 8426
E-mail: ieiblr@vsnl.com