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TRANSPORTATION FUEL FROM COAL WITH LOW CO_2 EMISSIONS

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Abstract

We present energy and carbon balances and cost estimates based on detailed Aspen Plus process simulations for five plant designs to co-produce dimethyl ether (DME) and electricity from coal. Four of the designs include capture of CO_2 for long-term underground storage. We also illustrate the potential DME offers for reducing emissions by facilitating a shift to more energy-efficient vehicles.

Introduction

Integrated gasification combined cycle (IGCC) technology offers the least costly approach to CO_2 capture and storage (CCS) for new bituminous coal power plants. Decarbonization via coal gasification can be extended to fuels used directly in transport, buildings, and industry, which account for 64% of global CO_2 emissions from fossil fuels.

One option is making H_2 from coal with CCS, which is expected to be the least costly option for providing H_2 with near-zero CO_2 emissions in a wide range of circumstances [1,2]. But because cost-competitive H_2 end-use technologies such as fuel cell vehicles will not be widely available for many years, H_2 cannot make major contributions in climate change mitigation until at least the second quarter of this century.

Coal gasification can also be used for synthetic liquid fuels manufacture—an option that is likely to get increasing attention in light of turmoil in the Middle East, where the world's remaining low-cost oil resources are concentrated. For example, China, with modest domestic oil resources, is intent on exploiting its vast coal resources to make synthetic liquid fuels from coal to help support its rapidly growing demand for transportation fuels [3]. Making liquid fuels from coal without capturing by-product CO_2 will lead to fuel-cycle CO_2 emissions that are up to double fuel-cycle emissions for petroleum-derived fuels, whereas fuel-cycle emissions with CCS can be less than for petroleum-derived fuels [4].

This paper explores a strategy for mitigating climate change for coal-derived synthetic fuels both by CCS and by choosing an energy carrier that facilitates a shift to more-efficient energy end-use technology. The focus is on dimethyl ether (DME). Its high cetane number makes DME a suitable candidate fuel for compression ignition engine vehicles, which are more energy efficient than spark-ignition engine vehicles. Compression ignition engine vehicles are not more widely used in part because of difficulties in realizing simultaneously low levels of emissions of both NO_x and particulate matter (PM), which are being sought in tightening air pollutant emission regulations throughout the world, driven by public health concerns. The tradeoffs that make simultaneous NO_x and PM control difficult for diesel fuel do not exist for DME, the combustion of which generates essentially no PM because of the absence of C-C bonds and of sulfur. Moreover, low NO_x emissions can be realized with much less complicated tailpipe emission control technologies. These pollution control advantages can facilitate a transition to fuel-efficient vehicles such as compression ignition engine/hybrid electric vehicles, although the pollution control advantages offered by DME are offset in part by the refueling infrastructure challenges that arise because at atmospheric pressure DME is a gas that must be stored in mildly pressurized canisters such as those required for LPG.

Building on previous work [4], we present energy and mass balances and cost analyses for several process designs for making DME from coal with alternative levels of carbon capture. All designs involve passing synthesis gas (syngas) only once through the synthesis reactor and making co-product electricity in a gas turbine/steam turbine combined cycle power plant—a configuration found to be typically more cost-effective than the alternative of recycling unconverted syngas to maximize fuel production [4]. The paper also illustrates the potential DME offers for reducing emissions by facilitating a shift to more energy-efficient vehicles.

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Process Designs

Coal is first gasified in oxygen in a Texaco type quench gasifier. The raw syngas is cooled, scrubbed, and passed through a sulfur-tolerant single-stage water gas shift (WGS) reactor to achieve the optimum H_2/CO ratio (1.0) for DME synthesis. An acid gas removal unit (AGR) removes H_2S (which would otherwise poison downstream catalysts) to ppb levels. It also removes most of the CO_2 in the gas to improve the yield of DME in the liquid-phase synthesis reactor following the AGR. (A small amount of CO_2 is required to maintain catalyst activity.)

Capture of CO_2 from the syngas upstream of the synthesis reactor is a low-cost partial decarbonization option. In DME manufacture, co-capture and co-storage of H_2S and CO_2 is a less costly acid gas management strategy than capturing the gases separately and reducing H_2S to elemental S while venting the CO_2 [4].

Further decarbonization can be realized in "once-through synthesis" designs, at higher cost, by adding additional shift reactors downstream of the synthesis reactor, recovering the CO_2 for geological storage, and using the CO_2-depleted, H_2-rich syngas to make electricity. When syngas is decarbonized both upstream and downstream of the synthesis reactor, it is possible to capture and store most of the carbon in the coal feedstock except that contained in the DME product.

Updating [4], we have developed five designs for co-producing DME and electricity. In one design (VENT), all CO_2 is vented. In a second design (UCAP), CO_2 is co-captured with H_2S in the upstream section of the plant, but no CO_2 is captured downstream of the synthesis island. In the last three designs (DCAP), CO_2 is co-captured upstream with H_2S (as in the UCAP case), and one or more shift reactors are deployed downstream of the synthesis reactor in alternative configurations to capture 85.1%, 89.0%, and 97.8% of the downstream CO_2 ($DCAP_{85}$, $DCAP_{89}$, and $DCAP_{98}$). The UCAP and DCAP cases have the same upstream configuration (Figure 1).

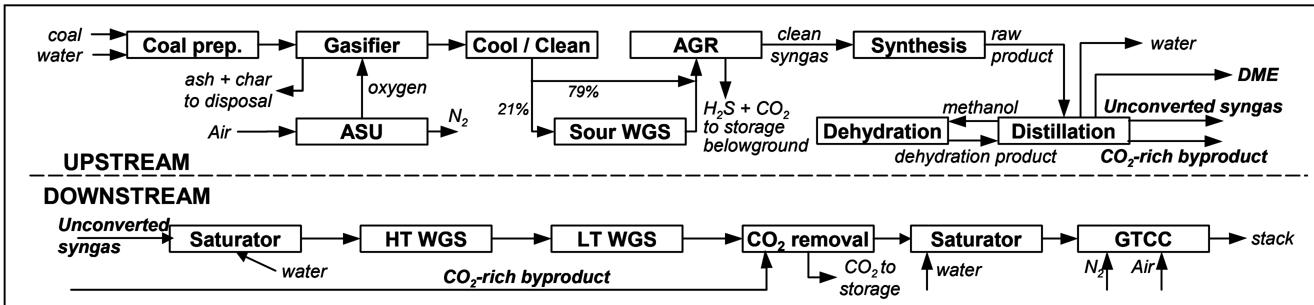

Figure 1. Simplified process diagrams. The upstream portion represents all cases except VENT. The downstream portion is for $DCAP_{98}$. Configurations for other cases are discussed in the text.

In contrast to earlier designs [4], we have *(i)* modeled the AGR as a Rectisol unit, which is more effective for deep sulfur removal than a Selexol unit; *(ii)* increased the fraction of CO_2 in the syngas going to the synthesis reactor from 1.75% to 3% by volume (there is uncertainty about what the required CO_2 fraction is); *(iii)* dehydrated the methanol by-product of DME synthesis in a separate reactor instead of recycling it to the synthesis reactor; *(iv)* improved the performance of the DME separation area to increase DME recovery; and *(v)* optimized upstream pressure drops, resulting in slightly higher operating pressure for the synthesis reactor. The net result of these updates to [4] is a 10% increase in the fraction of input coal converted to DME. Additionally, three streams leave the product separation area: DME (99.98% purity by mass), unconverted syngas, and a CO_2-rich byproduct of DME distillation (approximately 90% CO_2 by volume).

For the VENT and UCAP cases, the CO_2-rich distillation byproduct stream is mixed with the unconverted syngas and passed to a saturator where the gas picks up moisture before being burned in the gas turbine combined cycle. The humidification enables the syngas to be burned with acceptably low levels of NO_x generated.

In $DCAP_{98}$ (Figure 1), the unconverted syngas is passed first through a saturator to increase humidity to facilitate subsequent shifting of CO to H_2 via high- and low-temperature WGS reactors, after which the gas passes to a CO_2 removal unit. (The downstream and upstream Rectisol units share a solvent regenerator.) The CO_2-rich byproduct from the upstream product separation area bypasses the saturator and WGS reactors and goes directly to the Rectisol unit. Following CO_2 removal, the gas passes again through a saturator and then to the gas turbine. For the $DCAP_{89}$ case, 10% of the unconverted syngas is bypassed around the WGS and CO_2 removal units. For the $DCAP_{85}$ case, the second WGS reactor is removed, and there is no bypass around the WGS or Rectisol units. For all DCAP cases, some N_2 from the ASU is injected prior to the gas turbine combustor to help meet NO_x emission limits.

Energy and Carbon Balances

As in the earlier designs [4], each of our process schemes is designed to produce 600 MW (1795 tonnes/day) of DME from a bituminous coal from the Yanzhou area of Shangdong Province, China. In each case, 27.2% of the lower heating value of the input coal is converted to DME (Table 1). In the VENT case, the net electricity export is 490 MW. This decreases to 469 MW in the UCAP case, with further decreases in the DCAP cases. The parasitic electricity load increases with increasing fraction of carbon captured. The biggest added parasitic consumption in the DCAP cases is associated with the capture and compression of CO_2, but the compression of N_2 to meet NO_x constraints is also a significant added parasitic load. Overall, there is an efficiency penalty ranging from 4.5 to 5.5 percentage points for the DCAP cases relative to the UCAP case. The penalty for the UCAP case relative to the VENT case is 1 percentage point.

Table 1. Energy and carbon balances developed using Aspen Plus process simulation.

Energy Balance for Plant	VENT	UCAP	$DCAP_{85}$	$DCAP_{89}$	$DCAP_{98}$
Coal input, MW_{th} (LHV)	2203.1	2203.1	2203.1	2203.1	2203.1
Coal input, tC/hr	199.7	199.7	199.7	199.7	199.7
Total Internal power use, MW_e	137.4	159.2	222.2	224.8	233.7
Air separation unit	102.1	102.1	102.1	102.1	102.1
Coal handling and preparation	22.0	22.0	22.0	22.0	22.0
Acid gas removal and compression	3.12	24.9	59.3	60.9	64.5
Refrigeration	8.9	8.9	12.0	11.9	12.2
Nitrogen compression	0.0	0.0	23.3	24.1	28.9
Other auxiliary power uses*	1.3	1.3	3.4	3.7	4.0
Gas turbine gross output, MW_e	371.0	371.0	337.5	336.6	334.3
Steam turbine gross output, MW_e	256.8	256.8	251.8	253.2	251.9
Net power output, MW_e	490.3	468.6	367.1	365.0	352.5
DME output, MW_{th} (LHV)	600.2	600.2	600.0	600.0	600.0
Electric efficiency, % of coal LHV	22.3%	21.3%	16.7%	16.6%	16.0%
DME efficiency, % of coal LHV	27.2%	27.2%	27.2%	27.2%	27.2%
Total efficiency, % of coal LHV	49.5%	48.5%	43.9%	43.8%	43.2%
DME effective efficiency**	56.5%	54.0%	50.0%	49.8%	48.4%
Carbon Balance for Plant					
Total C buried as char, tC/h	2.0	2.0	2.0	2.0	2.0
Total C captured, excl. char, tC/h	-	57.5	143.5	147.6	156.4
% of Coal C: buried with ash (char)	1.0%	1.0%	1.0%	1.0%	1.0%
Co-removed upstream with H_2S	0.0%	28.8%	28.8%	28.8%	28.8%
Removed from gas downstream	0.0%	0.0%	43.1%	45.1%	49.5%
Vented at upstream AGR unit	28.8%	0.0%	0.0%	0.0%	0.0%
Vented from power island	50.6%	50.6%	7.6%	5.6%	1.1%
Carried in DME product	19.6%	19.6%	19.6%	19.6%	19.6%
Total C captured, % of coal C	1.0%	29.8%	72.9%	74.9%	79.3%

* Power for several small compressors less the output of a syngas expander.
** Defined as $D / [C - (E / eff)]$, where D is the LHV of DME output, C is LHV of coal input, E is net electricity output, and *eff* is the efficiency of a stand-alone coal-IGCC as given in Table 2. For the VENT and UCAP cases, *eff* is the value under "Vent CO_2". For the DCAP cases, *eff* is the value under "Capture CO_2".

For the UCAP and DCAP cases, approximately 30% of the carbon in the input coal is captured in the upstream portion of the plant, and 20% is carried in the DME leaving the plant (Table 1). Varying fractions of the remaining carbon are emitted in the gas turbine exhaust. How these emissions are allocated between the two co-products of the plant is arbitrary. Here, we allocate to electricity the fuel cycle GHG emission rates for stand-alone IGCC plants

Table 2. Characteristics of stand-alone coal-IGCC power plants.*

	Vent CO_2		Capture CO_2	
Coal price, \$/GJ$_{LHV}$ →	0.5	1.0	0.5	1.0
Installed capacity, MW_e	390.1		359.9	
Overnight installed cost, \$/kW	1187		1461	
Efficiency, % LHV	42.95		36.58	
Total generating cost, \$/kWh	0.0397	0.0441	0.0529	0.0580
Fuel cycle GHG emissions, gC_{equiv}/kWh	217.3		20.40	

* Capacity, costs, and efficiency are for EVQ (CO_2 vented, Quench) and ECQ (CO_2/H_2S co-capture/co-storage) cases in [7,8], but with indicated coal price. Emissions are for indicated efficiencies, but Yanzhou coal [4] and assume 1 $kgC_{equiv}/GJ_{coal\ LHV}$ from coal mining/transport.

Table 3. Carbon emissions accounting.

System GHG Emissions per kWh Electricity	VENT	UCAP	$DCAP_{85}$	$DCAP_{89}$	$DCAP_{98}$
From coal mining/transport, gC_{equiv}/kWh	16.2	16.9	21.6	21.7	22.5
From AGR area, gC/kWh	117.3	0.0	0.0	0.0	0.0
From power island, gC/kWh	206.3	215.8	41.2	30.4	6.3
Total emissions, gC_{equiv}/kWh	339.7	232.8	62.8	52.1	28.8
Emissions assigned to electricity, gC_{equiv}/kWh	217.3	217.3	20.4	20.4	20.4
Plant+upstream DME emissions, $kgC_{equiv}/GJ_{DME\ LHV}$	27.8	3.4	7.2	5.4	1.4
DME end use emissions, $kgC/GJ_{DME\ LHV}$	18.1	18.1	18.1	18.1	18.1
Total DME-related emissions, $kgC_{equiv}/GJ_{DME\ LHV}$	45.9	21.4	25.3	23.4	19.5
Fuel-cycle diesel fuel emissions, $kgC_{equiv}/GJ_{diesel\ LHV}$	26.1	26.1	26.1	26.1	26.1

(Table 2). In the VENT and UCAP cases, where there is no downstream decarbonization (i.e., no electricity decarbonization), we assign to electricity the emissions for an IGCC with no carbon capture. For the DCAP cases, we assign to electricity the emissions for an IGCC in which approximately 96% of the CO_2 is captured.

Our lifecycle accounting, which includes GHG emissions of 1 $kgC_{equiv}/GJ_{coal\ LHV}$ associated with activities upstream of the coal conversion facility, is summarized in Table 3. Emissions charged to electricity in the VENT and UCAP cases are 217 gC_{equiv}/kWh. In the DCAP cases, they are 20 gC_{equiv}/kWh. The balance of emissions are charged against DME production. Together with the intrinsic carbon in the DME, the fuel cycle GHG emissions of DME total 46 kgC_{equiv}/GJ in the VENT case and range from 20 to 25 kgC_{equiv}/GJ in the other cases. For comparison the fuel cycle-wide GHG emission rate is 26 kgC_{equiv}/GJ for crude oil-derived diesel fuel. Figure 2 shows the distribution of assigned GHG emissions per GJ of coal input.

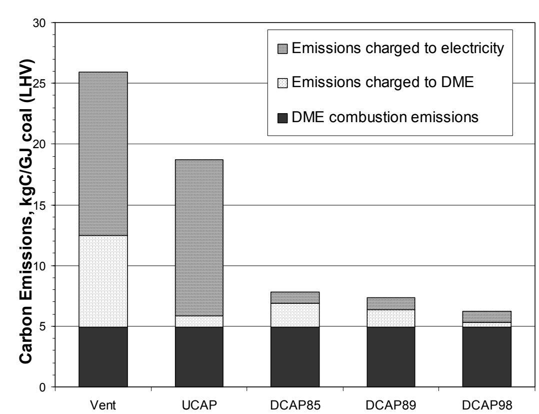

Figure 2. Distribution of GHG emissions charged to electricity and to DME, including CO_2 emissions at the plant and associated with DME combustion, as well as GHG emissions associated with activities upstream of the conversion plant. GHG emissions associated with activities downstream of the conversion plant are not included. See Table 3.

Costs

Following [4], capital costs are estimated for DME-electricity co-production facilities built at a generic United States' location (Table 4, upper section). Consistent with the results of [4], the installed capital cost is lower for the UCAP than for the VENT case, despite the fact that CO_2 is captured in the former case but not in the latter. This results from cost savings in co-capturing H_2S and CO_2 in the AGR in the UCAP case, which requires only a single Rectisol absorber column compared to capturing only H_2S in the VENT case, which requires two absorbers to separately remove H_2S and CO_2 from the syngas (even if the CO_2 is subsequently vented). In addition, the VENT case requires Claus and SCOT plants to recover elemental sulfur from H_2S. These cost differences are partly offset by the absence of CO_2 compression requirements in the VENT case.

We estimate levelized costs of DME production (assuming 12.4% interest during construction, 15% annual capital charge rate, and 80% plant capacity factor) for coal prices of $1/GJ$_{LHV}$ and $0.5/GJ$_{LHV}$, representing a city-gate location and a mine-mouth location. We assume that by-product electricity would be valued at the cost of generating electricity in stand-alone IGCC systems paying the same price for coal and venting all carbon (VENT and UCAP cases) or co-capturing/co-storing H_2S and 96% of CO_2 (DCAP cases). See Table 2.

Table 4. Capital cost estimates and levelized lifecycle costs of DME production.

	VENT	UCAP	DCAP$_{85}$	DCAP$_{89}$	DCAP$_{98}$
Overnight Installed Capital Costs (million 2003 $)					
Coal storage, preparation, handling	92.80	92.80	92.80	92.80	92.80
Gasifier (4 trains)	190.24	190.24	190.24	190.24	190.24
Air separation (2 trains)	103.28	103.28	103.28	103.28	103.28
Upstream WGS area	10.35	10.35	10.35	10.35	10.35
Rectisol (upstream + downstream)	80.91	44.95	54.52	54.10	55.02
CO_2 drying and compression	-	21.30	38.31	39.03	40.54
Sulfur Recovery (Claus, SCOT)	55.82	-	-	-	-
DME synthesis	26.46	26.46	26.46	26.46	26.46
DME distillation	44.21	44.21	44.20	44.20	44.20
Methanol dehydration	1.69	1.69	1.69	1.69	1.69
Syngas expander	1.69	1.69	1.69	1.69	1.69
Downstream WGS area	-	-	19.18	44.69	47.96
Saturators	0.25	0.25	0.41	0.39	0.40
Fuel gas compressor	-	-	2.49	2.72	2.92
N_2 compressor	-	-	8.41	8.62	9.72
Other capital costs	3.01	2.84	2.85	2.80	2.81
Fuel area BOP	91.61	81.01	89.53	93.46	94.51
Gas turbine	108.40	108.40	100.98	100.78	100.26
Steam turbine and HRSG	113.82	113.81	112.33	112.74	112.36
Power island BOP	73.18	73.18	70.14	70.18	69.89
Total overnight capital cost	997.73	916.49	969.88	1000.22	1007.10
Levelized Cost of DME ($/GJ, 2003$) (80% capacity factor, 12.4% construction interest)					
15% of total capital/year	11.11	10.02	10.80	11.14	11.22
O&M (4% of overnight capital/year)	2.64	2.42	2.56	2.64	2.66
Acid gas transport and storage ($5/t)	0.00	0.52	1.24	1.28	1.35
Subtotal	13.75	13.14	14.61	15.06	15.23
For coal price = $1/GJ					
Coal feedstock	3.67	3.67	3.67	3.67	3.67
Electricity (revenue)	-10.01	-9.57	-9.86	-9.80	-9.46
Total net DME cost, $/GJ$_{LHV}$	**7.41**	**7.25**	**8.42**	**8.93**	**9.44**
$/liter diesel equivalent	**0.27**	**0.26**	**0.30**	**0.32**	**0.34**
For coal price = $0.5/GJ					
Coal feedstock	1.84	1.84	1.84	1.84	1.84
Electricity (revenue)	-9.01	-8.61	-8.99	-8.94	-8.63
Total net DME cost, $/GJ$_{LHV}$	**6.57**	**6.37**	**7.45**	**7.96**	**8.43**
$/liter diesel equivalent	**0.24**	**0.23**	**0.27**	**0.29**	**0.30**

The lower section of Table 4 gives the resulting levelized costs of DME. For the VENT case, the estimated DME cost ranges from $6.6/GJ to $7.4/GJ over the coal cost range considered. This corresponds to $0.24/liter of diesel equivalent (lde) to $0.27/lde. The UCAP case gives a slightly lower DME cost, for reasons discussed earlier. In the DCAP cases, the DME costs are higher, but in all cases are below $0.35/lde.

In the early years, synfuel production will be concentrated at sites with low-cost coal. For $0.5/GJ coal, the crude oil price at which wholesale prices are equal for DME and diesel fuel ranges from $27 to $36 per barrel ($30 per barrel for the $DCAP_{85}$ case)—when CO_2 emissions are valued at $0/tC for the VENT/UCAP cases and $67/tC (the avoided cost for the IGCC with CCS compared to IGCC with CO_2 vented) for the DCAP cases . Such surprisingly low DME production costs must be considered together with extra costs of getting DME to the consumer (infrastructure costs) relative to petroleum diesel and potentially lower costs for DME vehicles as a result of lower costs for pollution controls. A preliminary analysis suggests that added infrastructure costs may be roughly offset by the reduced vehicle costs [5].

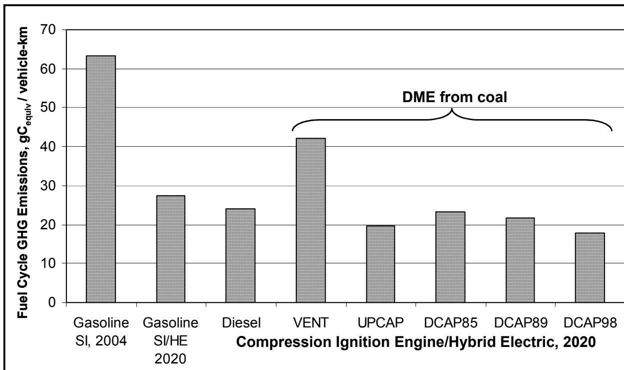

Figure 3. Fuel-cycle GHG emissions, including feed-stock (crude oil or coal) extraction and transport to conversion plant, fuel conversion, and fuel combustion. For gasoline and diesel fuel, emissions associated with fuel delivery to the car (based on GREET model) are also included. The 6 bars on the right are for a CIE/HE car in 2020.

Potential Impact on Transportation Sector CO_2 Emissions

Weiss, *et al.* [6] project that by 2020 (at which time it is conceivable that DME could be established in automotive markets), new compression ignition engine/hybrid electric (CIE/HE) cars with performance equivalent to that for today's 7.9 liters/100 km [30 miles per gallon (mpg)] gasoline cars could achieve a fuel economy of 2.8 liters gasoline equivalent (@ 31.4 MJ/liter) per 100 km (80 mpg_{ge}). Using DME made with CCS in such cars would lead to a fuel cycle GHG emission rate per km that is 75-97% of that for diesel fuel used in such cars and 27-36% of the rate for today's 7.9 l/100 km (30 mpg) gasoline cars (Fig. 3).

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