IS THERE ROOM IN THE ATMOSPHERE FOR COAL SYNFUELS?

OPPORTUNITIES FOR CO_2 CAPTURE/STORAGE AND END-USE EFFICIENCY GAIN

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Carbon Capture and Separation
GCEP Energy Workshop
Global Climate and Energy Project
Stanford University
27 April 2004

Acknowledgments

- The findings reported are fruits of a research collaboration exploring coal polygeneration technologies and strategies, with focussed attention on applications in China:
  - Tsinghua University: Li Zheng, Ren Tingjin, Ni Weidou
  - Princeton University: Eric Larson, Bob Williams

- Princeton research supported by:
  - Princeton’s Carbon Mitigation Initiative (BP, Ford)
  - Hewlett Foundation, Packard Foundation, Blue Moon Fund, National Commission on Energy Policy

WHY CLEAN SYNFUELS FROM COAL IN CLIMATE-CONSTRAINED WORLD

- Oil supply concerns
  - Oil supply insecurity
  - Peaking of conventional oil production…before 2025?
  - Rapid transport demand growth, scant domestic oil
    - ➔ strong coal synfuels interest in China
- H_2 FCVs cannot make major transportation contributions

  until 2nd Qtr 21st century
- Clean “designer” fuels can facilitate shift to more efficient (CI) engine vehicles (*by reducing requirements for tailpipe emission controls*)
- Black carbon issue for conventional Diesel
- Potential GHG mitigation benefits with CCS relative to crude-oil derived transport fuels
- Early opportunities for CCS (*even before climate policy enacted*) via CO_2/H_2S co-capture/co-storage as acid gas management strategy

H_2 + NEW CARBON-BASED ENERGY CARRIER?

- Optimistic scenario for new H_2 FCV production:
  - *2005-2009*: 10,000 FCVs/y in pilot manufacturing facility.
  - *2010*: 300,000 FCVs in first commercial factory.
  - *Beginning 2013*: Many aggressive (~ *50%*) ZEV mandates
  - *2013-2019*: 3 new 300,000 FCVs/y factories added annually
  - 2020-2025: 10 new 300,000 FCVs/y factories added annually

➔130 million H_2 FCVs (*11% of global car population*) by 2025 (*20% of new cars*)—global emissions reduction rate = 0.1 GtC/y

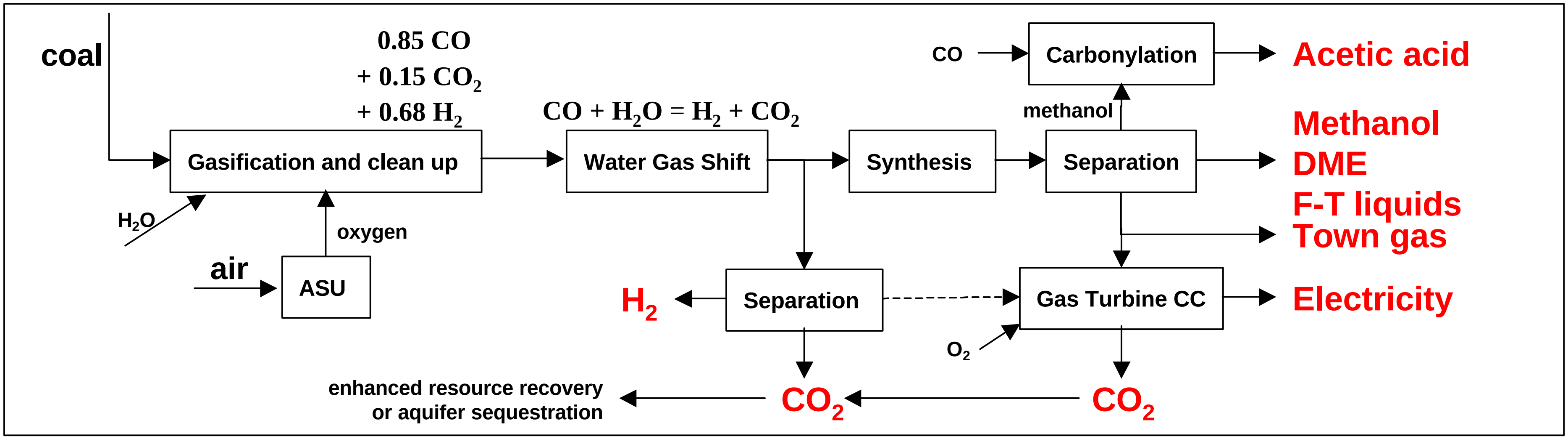
➔Need complementary AP, GHG, OSI mitigation strategy for cars in 1st Qtr of 21st century

LIQUID FUELS FROM COAL

Challenge: increase H/C ratio (*H/C ~ 2 for HC fuels; ~ 0.8 for coal*)

- Gasify coal in O_2/H_2O to produce “syngas” (*mostly CO*, H_2)
- Increase H/C ratio via WGS to maximize conversion in synthesis reactor ($CO + H_2O \rightarrow H_2 + CO_2$)
- Remove acid gases (H_2S *and* CO_2), other impurities from syngas
- Convert syngas to synthetic fuel in “synthesis” reactor
- Can strive to make fuels superior to crude oil-derived HC fuels:
    (*i*) set goals for performance, air-pollutant emissions, cost;
    (*ii*) seek chemical producible from CO, H_2 that comes closest to meeting goals;
    (*iii*) develop that chemical (*“designer fuel” strategy*)

Coal polygeneration – general scheme



coal

0.85 CO
+ 0.15 CO_2
+ 0.68 H_2

Gasification and clean up

H_2O

oxygen

air

ASU

$CO + H_2O = H_2 + CO_2$

Water Gas Shift

Synthesis

CO

Carbonylation

methanol

Separation

Acetic acid

Methanol
DME
F-T liquids
Town gas

H_2

Separation

Gas Turbine CC

Electricity

O_2

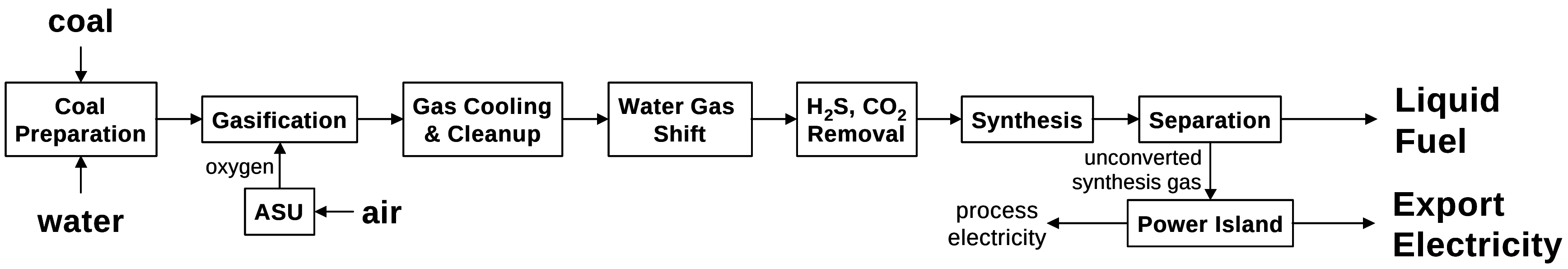
enhanced resource recovery
or aquifer sequestration

CO_2

CO_2

Co-production of synfuel and electricity (*or multiple products*) will often be favored. This "polygeneration" concept is "taking off" at refineries, chemical process plants worldwide and may soon be introduced for the production of synfuels (*China is the country to watch*). Producing high H/C ratio fuels from coal ➔ relatively pure CO_2 coproduct and low cost CO_2 capture costs for CO_2 captured prior to fuel synthesis.

ONCE-THROUGH (OT) vs RECYLE (RC) OPTIONS



coal

water

Coal Preparation

Gasification

oxygen

ASU

air

Gas Cooling & Cleanup

Water Gas Shift

H_2S, CO_2 Removal

Synthesis

Separation

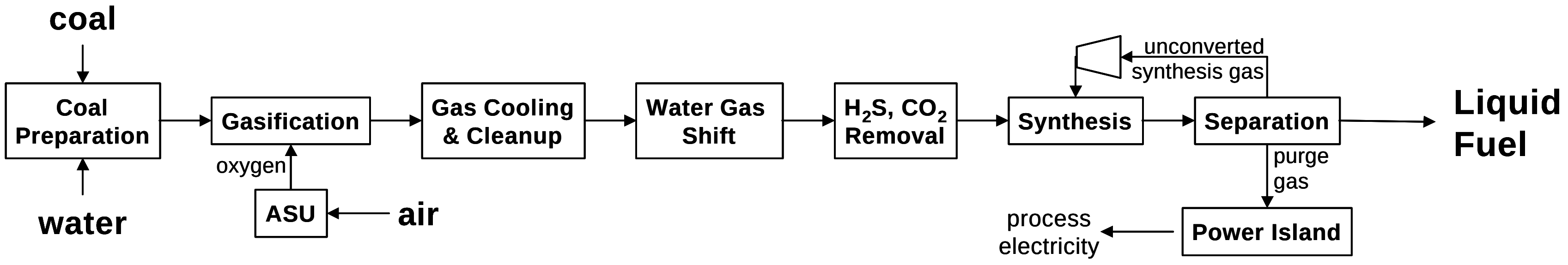
unconverted synthesis gas

Power Island

process electricity

Liquid Fuel

Export Electricity



coal

water

Coal Preparation

Gasification

oxygen

ASU

air

Gas Cooling & Cleanup

Water Gas Shift

H_2S, CO_2 Removal

Synthesis

unconverted synthesis gas

Separation

purge gas

Power Island

process electricity

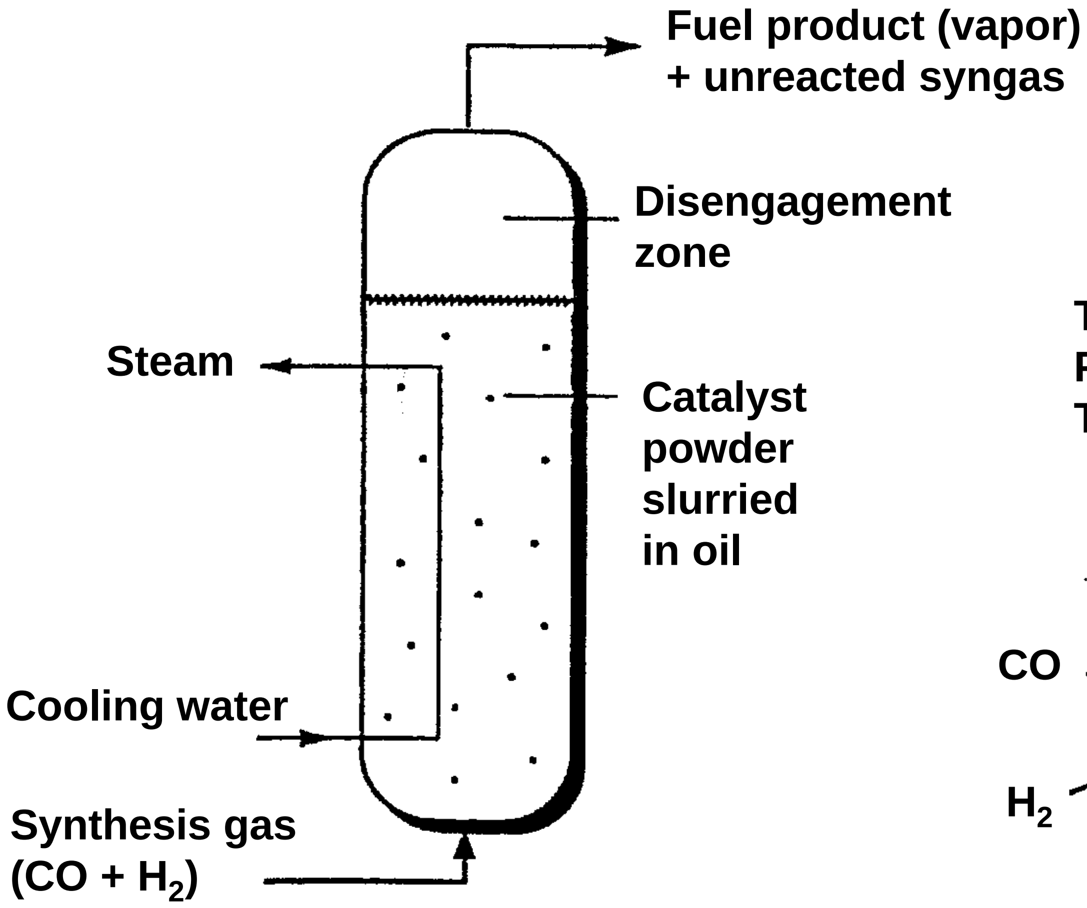
Liquid Fuel

- <u>OT option</u> (*top*): syngas passes once through synthesis reactor; unconverted syngas burned → electricity coproduct in combined cycle
- <u>RC option</u> (*bottom*): unconverted syngas recycled to maximize synfuel production; purge gases burned → electricity for process; no electricity export
- OT systems especially attractive when using liquid-phase reactors

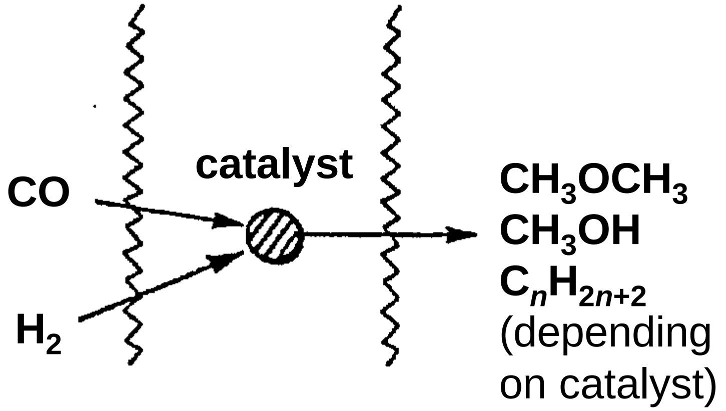
Liquid-Phase (LP) Synthesis Technology

Well-suited for use with
CO-rich (coal-derived) syngas

Liquid-phase reactors have much higher one-pass conversion of $CO+H_2$ to liquids than traditional gas-phase reactors, e.g., liquid-phase Fischer-Tropsch synthesis has ~80% one-pass conversion, compared to <40% for traditional technology.



TYPICAL REACTION CONDITIONS:
P = 50-100 atmospheres
T = 200-300°C



Status of LP Synthesis Technology

	Fischer-Tropsch	MeOH	DME
Commercial units in operation	✓		
Demonstrated at commercial scale		✓	
Demonstrated at pilot-plant scale			✓

ICL PROCESS DESIGN AND SIMULATION

AspenPlus™ process software used by Princeton/Tsinghua team to design and simulate performance of ICL systems for coal-derived methanol and DME with different equipment configurations:

- **Once-Through** with CO_2
  - (1) Vented
  - (2) Captured and compressed for pipeline → storage
  - (3) Captured and compressed together with H_2S for pipeline → storage
- **RECYCLE** with CO_2
  - (1) Vented
  - (2) Captured and compressed for pipeline → storage
  - (3) Captured and compressed together with H_2S for pipeline → storage

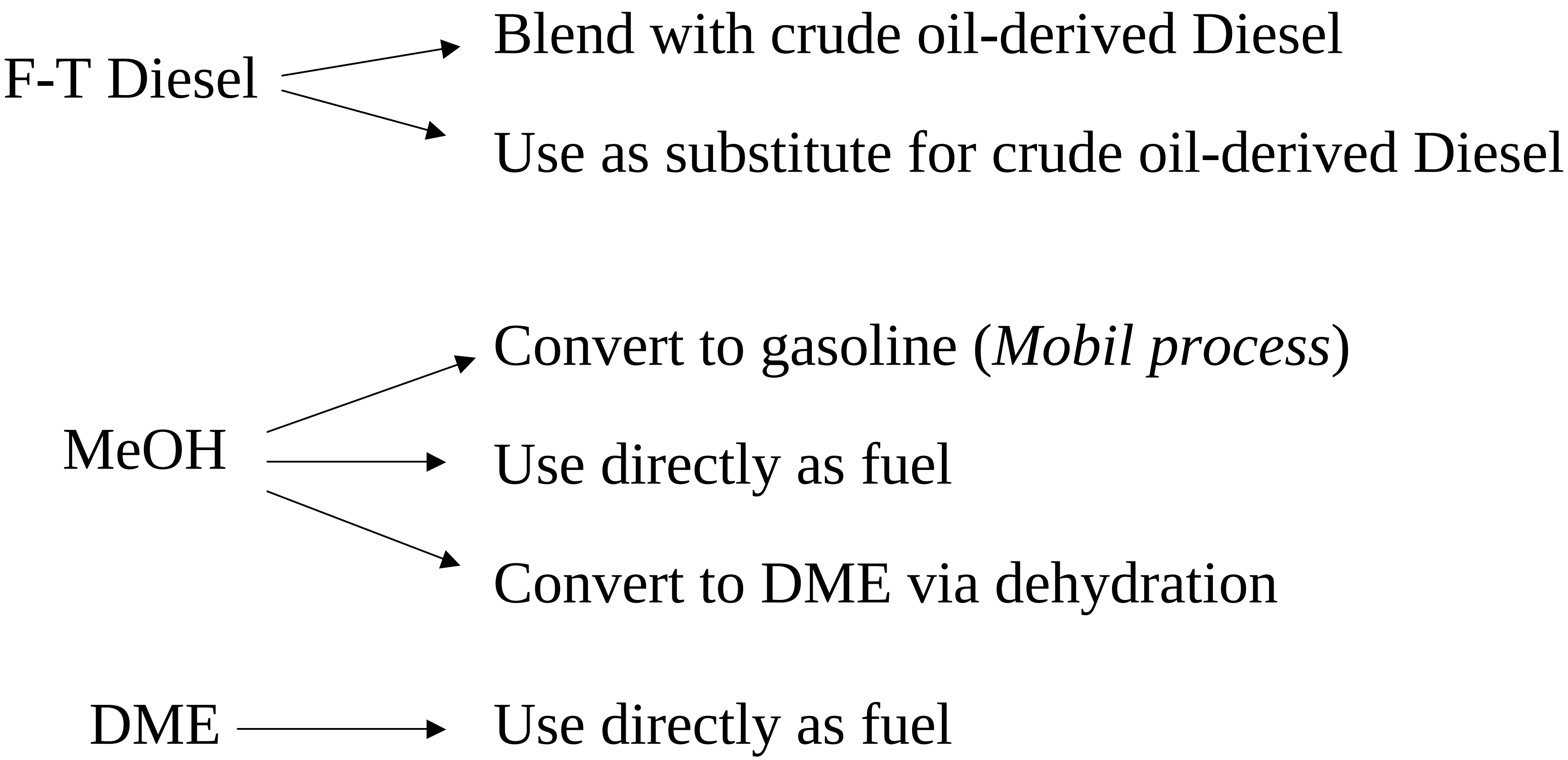
Performance results verified through literature review and communication with industry experts.

PARAMETERS FOR ESTIMATING COSTS FOR SYNFUEL PRODUCTION VIA ICL

- Interest during construction = 16% of overnight capital cost.
- Annual capital charge rate = 15%.
- Annual capacity factor = 85%.
- Non-fuel operating & maintenance cost = 4% of overnight capital cost.
- Coal cost
  - $1/GJ (*$23.5/tonne, as received*) for city-gate plant
  - $0.5/GJ for minemouth plant
- Reference electricity sale price = $0.043/kWh for coal @ $1/GJ

  (*IGCC electricity cost estimated using same basic assumptions as for ICL*)
- CO_2 pipeline and underground injection cost ranges from $4.7-8.5 per tCO_2 (*based on Ogden model*).

SYNFUEL OPTIONS VIA COAL GASIFICATION



F-T Diesel
- Blend with crude oil-derived Diesel
- Use as substitute for crude oil-derived Diesel

MeOH
- Convert to gasoline (*Mobil process*)
- Use directly as fuel
- Convert to DME via dehydration

DME
- Use directly as fuel

DME (CH_3OCH_3)

- Ozone-safe aerosol propellant and chemical feedstock.
- Production ~ 150,000 t/y by MeOH dehydration (*small plants*)
- Good CIE fuel: high cetane #, no sulfur, no C-C bonds that could lead to soot ➔ no PM/NO_x tradeoff in quest for low emissions—low NO_x emissions; solves black carbon problem
- Properties as cooking fuel are similar to propane or LPG

PROPERTIES	**DME**	**Propane**	**Diesel Fuel**
Boiling point, ^{o}C	-24.9	-42.1	180 – 370
Vapor pressure, atm.	5.1	8.4	<< 1
Liquid density, kg/m^3	668	501	~ 840
Liquid lower heat value, MJ/kg	28.4	46.0	42.5
Flammability limits in air, vol%	3.4 – 17	2.1 – 9.4	0.6 – 6.5
Auto-ignition temperature (^{o}C)	235	470	250
Cetane number	55 – 60	5	40 – 55

WILL F-T DIESEL AND DME BECOME MAJOR FOCI OF SYNFUELS DEVELOPMENT?

- For transport, synfuel emphasis likely to be on CIE fuels
  - Both F-T Diesel and DME outstanding for these uses
  - No new infrastructure requirement ➔F-T Diesel can be introduced much more quickly (*in Diesel blends*) than neat DME ➔ quicker impact in reducing oil import dependency for transport.
  - F-T Diesel likely to have major role in blends as long as crude oil-derived Diesel has major presence in world market.
  - DME offers outstanding AP, BC benefits…but requires infrastructure change
  - DME transport infrastructure challenge not so daunting for China
- DME likely to play major role as clean fuel for rural areas of developing countries…as LPG supplement to replace highly polluting coal and biomass fuels for cooking/heating

Single-Step DME synthesis

$CO + 2H_2 \Leftrightarrow CH_3OH$ (MeOH synthesis) - 91 kJ/mol

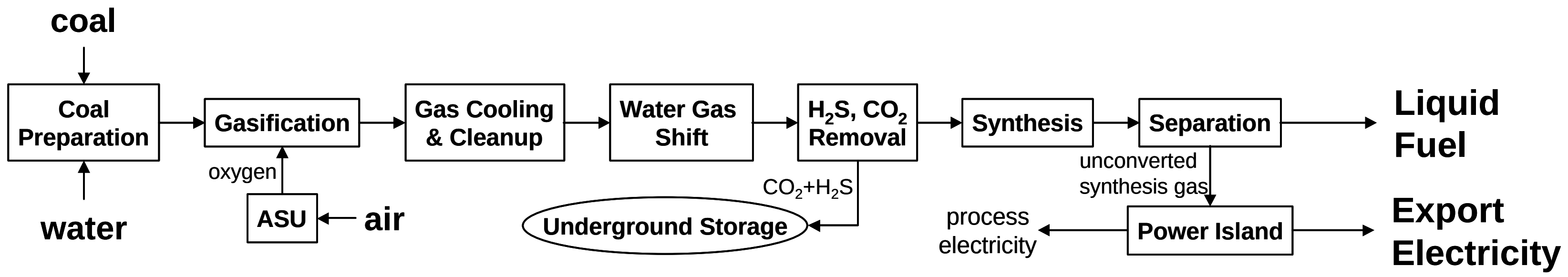
$2CH_3OH \Leftrightarrow CH_3OCH_3 + H_2O$ (dehydration) - 24 kJ/mol

$H_2O + CO \Leftrightarrow H_2 + CO_2$ (water gas shift) - 41 kJ/mol

- One original motivation for DME: higher conversion feasible than with MeOH (*MeOH formation is equilibrium limited but dehydration removes MeOH as it forms, enabling equilibrium limit to be surpassed*).
- Two catalysts suspended in oil of synthesis reactor
  - $CuO/ZnO/Al_2O_3$ for MeOH synthesis, WG
  - γ-alumina for MeOH dehydration

CO_2 CAPTURE & STORAGE

FOR ACID GAS MANAGMENT



coal

Coal Preparation

water

Gasification

oxygen

ASU

air

Gas Cooling & Cleanup

Water Gas Shift

H_2S, CO_2 Removal

CO_2+H_2S

Underground Storage

Synthesis

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unconverted synthesis gas

Liquid Fuel

Power Island

process electricity

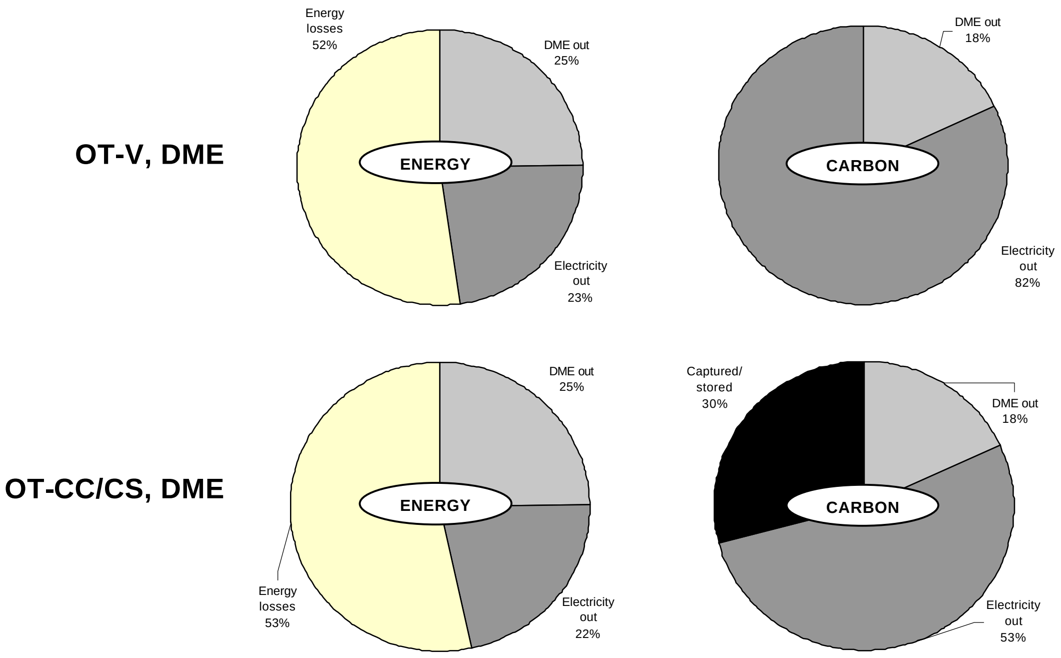
Export Electricity

Acid gas (H_2S + CO_2) management:

- –H_2S level in syngas must be reduced to ppbv levels to protect synthesis catalysts
- – ~ 95% of CO_2 should be removed to maximize syngas conversion to synfuel

H_2S/CO_2 co-capture/co-storage (CC/CS) often less costly than separate CO_2 and H_2S removal + conversion, $H_2S \rightarrow S$.

ENERGY/CARBON BALANCES FOR DME/ELECTRICITY CO-PRODUCTION SYSTEMS



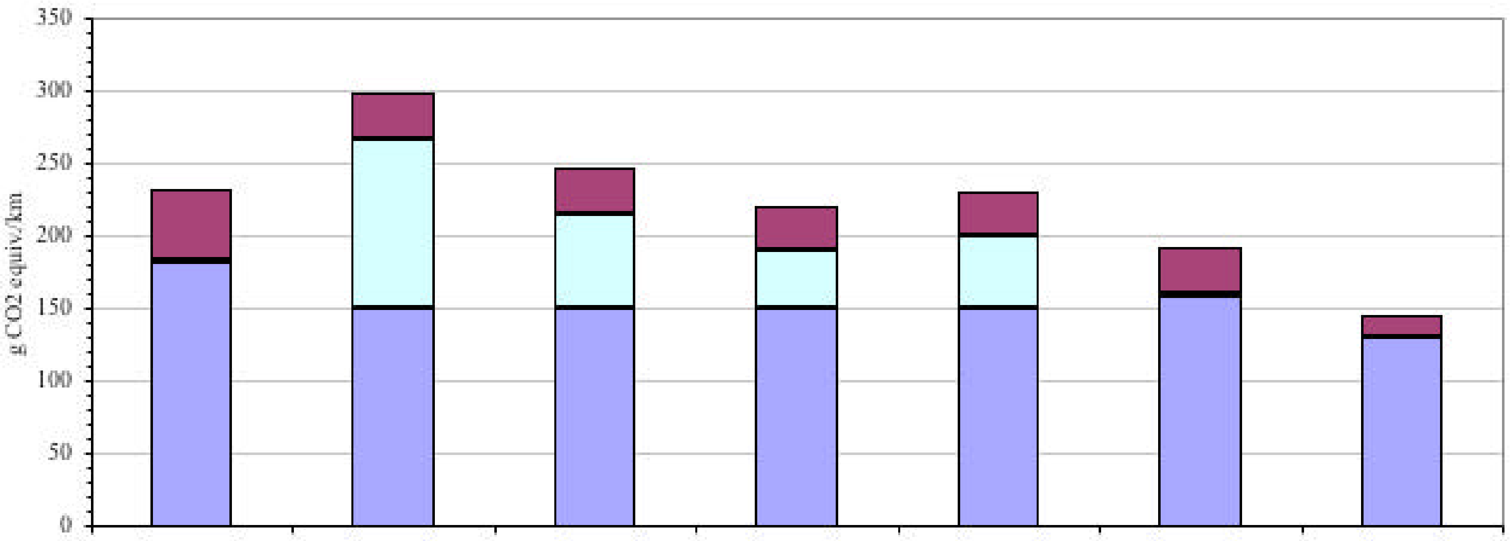
- Consider OT-CC/CS @ 526 MW_e, 600 MW DME
  - CO_2 storage @ 1.8 x 10^6 t/y & storage @ \$6/t CO_2
  - DME cost = 0.95 x DME cost for OT-V case
- Fuel cycle GHG emission rate for OT-CC/CS case:

Electricity: same as for 40%-efficient coal power plant venting CO_2

DME: 0.8 X rate for Diesel from crude oil

FUEL CYCLE EMISSIONS FOR GLOBAL WARMING

(*Alternative Engine/Fuel Combinations For Cars*)



Regulation	Tier II (US 2004+)	Euro I (India 2000)	Euro II (India 2005)	Euro III (Europe 2000)	Tier I (US 1997)	Tier II (US 2004+)	Tier II (US 2004+)
Engine	SIE	CIE	CIE	CIE	CIE	CIE	CIE
Fuel	RFG	Diesel	Diesel	Diesel	Diesel	Low S Diesel	DME w/CCS
Primary Energy	Petroleum	Petroleum	Petroleum	Petroleum	Petroleum	Petroleum	Coal
Fuel Economy	30 mpg	38 mpg_{ge}	38 mpg_{ge}	38 mpg_{ge}	38 mpg_{ge}	36 mpg_{ge}	38 mpg_{ge}

1 g Diesel PM ≡ 870 g CO_2, net BC global warming (Delucchi, 2003)

Acronyms

RFG = Reformulated Gasoline
SIE = Spark Ignition Engine
CIE = Compression Ignition Engine
CCS = Carbon Capture and Storage

CHALLENGES IN MEETING TIER II STANDARDS FOR CIE VEHICLES (*OR EQUIVALENT*)

- High costs for compliance ~ \$500 per car
- Rapidly industrialized countries will want Diesel cars (*to help limit oil import dependence*)…but will they be willing to pay cost for reducing emissions to level needed to comply with Tier II standards?
- Even if eventually AP controls prove to be affordable, there is strong chance that actual emissions will exceed standard, on average
- Compliance costs reduced modestly with shift to F-T Diesel
- Compliance costs reduced substantially with shift to DME…and non-compliance risk modest

DME/DIESEL COMPETITION IN CARS—US vs CHINA
(*POLYGENERATED COAL DME, 38 mpg_{ge} DME cars*)

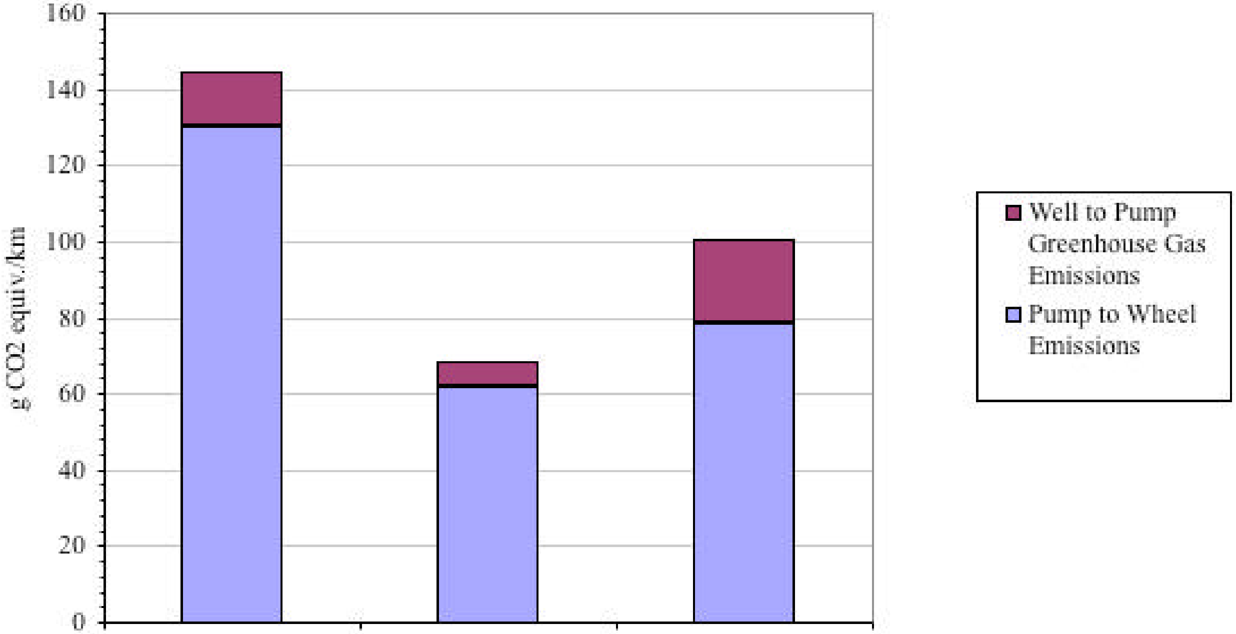
	US	China
Annual driving (km)	19,300	14,000
Total capital for plant	$\$1.4 \times 10^9$	$\$1.0 \times 10^9$
DME cost ($/gallon Diesel equiv)	$0.98/gal	$0.76/gal
	Breakeven crude oil price ($/bbl)	
If DME car cost = Diesel car cost	38	31
If DME car costs $340 less	30	21
Above + $100/tC carbon tax	26	17

For minemouth plants *($0.5/GJ coal)* making 526 MW_e electricity + 600 MW DME (*9,100 b/d of Diesel equivalent*) with CO_2/H_2S co-capture and co-storage

Fuel distribution cost increment for DME = $0.20/gallon Diesel equivalent

FUEL CYCLE EMISSIONS FOR GLOBAL WARMING

(*Alternative Engine/Fuel Combinations For Cars*)



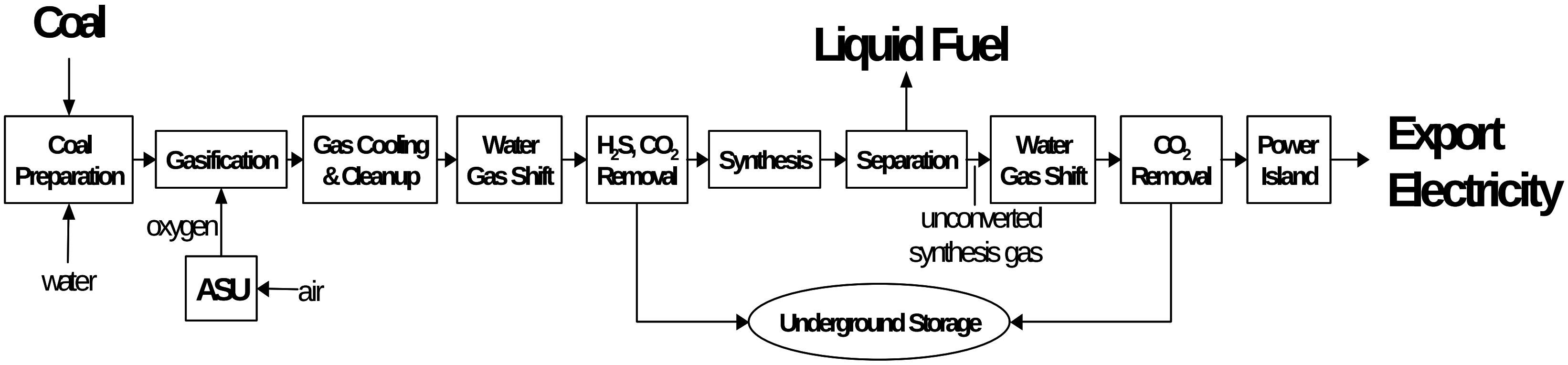
Regulation	Tier II (US 2004+)	Tier II (US 2004+)	Tier II (US 2004+)
Engine	CIE	CIE/HE	SIE/HE
Fuel	DME w/CCS	DME w/CCS	RFG
Primary Energy	Coal	Coal	Petroleum
Fuel Economy	38 mpg$_{ge}$	80 mpg$_{ge}$	69 mpg$_{ge}$

Acronyms

RFG = Reformulated Gasoline
SIE = Spark Ignition Engine
CIE = Compression Ignition Engine
HE = Hybrid Electric
CCS = Carbon Capture and Storage

With DME shift, CIE → CIE/HE (*80* mpg_{ge}), CO_2 equiv emissions
→ ~ 1/3 of level for today's SIE cars (*30 mpg*)
2/3 of level for gasoline SIE/HE (*69 mpg)*

Under Climate Policy Co-Produce DME/Electricity with CO_2 Capture Ahead Of + After Synthesis Reactor


Coal
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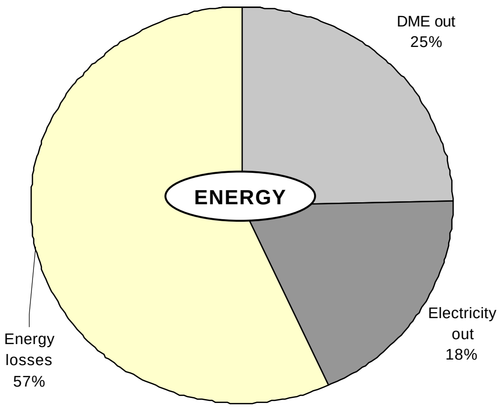
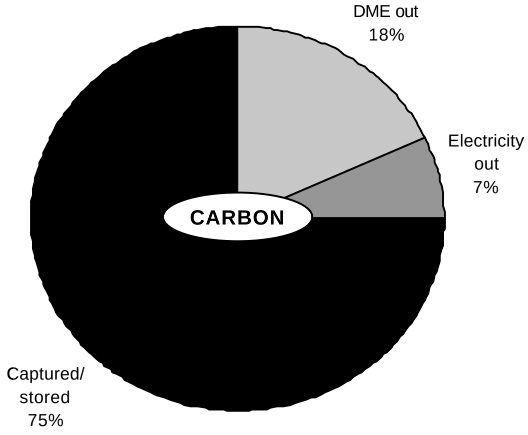


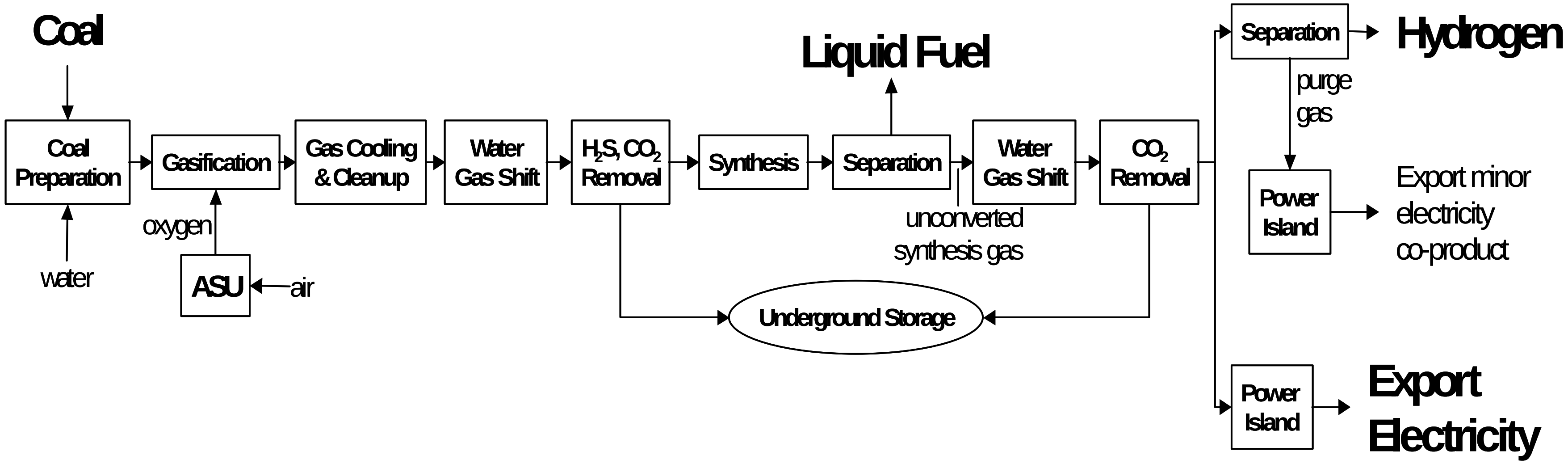


Fuel cycle GHG emission rate:

<u>Electricity</u>: ~ 0.2 X rate for 40%-efficient coal plant (*CO_2 vented*)

<u>DME</u>: ~ 0.8 X rate for Diesel from crude oil (*same as before*)

Decarbonized Coal Energy Coproduction in Long Term



By the time H_2 is launched in market as energy carrier:

- Decarbonized syngas downstream of liquid fuel synthesis reactor can be used to produce mix of electricity + H_2
- H_2/electricity output ratio would be determined mainly by relative H_2/electricity market demands because system efficiencies/costs invariant over wide range of H_2/electricity output ratios

IRR ANALYSIS OF DME/ELECTRICITY

CO-GENERATION FOR CO_2 STORAGE DEMOS

Plant capital cost relative to base case	CO_2 Selling Price ($/t)	IRR on equity
1.0	10	17.8
1.0	15	18.8
1.0	20	19.7
1.2	20	16.0

Common assumptions for all cases:

- 600 MW DME, 536 MW_e electricity, US construction
- 1.8 x 10^6 t/y CO_2 available for demos (or EOR) 100 km from plant
- Financing:
  - 55%/45% debt/equity; debt @ 6.5%/y interest; 2%/y inflation
  - 20 y tax life, 30 y book life; 2%/y PTI; 4 y construction
- DME price = refinery-gate Diesel cost for $25/bbl WOP
- Electricity price = $0.04/kWh
- Coal price = $0.5/GJ (*minemouth plant*)

SUMMING UP THE CASE FOR GIVING SERIOUS ATTENTION TO CCS FOR COAL SYNFUELS

- Powerful motivations for making clean synfuels from coal
  - Oil supply insecurity mitigation
  - Ultra-low air pollutant and black carbon emissions for “designer fuels”
  - Potentially attractive economics via polygeneration
- Without CCS, coal synfuels would be disastrous for climate
- With CCS coal synfuels can be more climate-friendly than crude oil derived fuels
- Designer fuels can facilitate introduction of more efficient engines in transport
- Can get early (*pre-climate-mitigation policy*) experience with CO_2 storage pursuing CC/CS as acid gas management strategy…but this finding contingent on viability of H_2S/CO_2 co-storage
- Coal synfuels provided via polygeneration offer evolutionary coal processing framework for transition to coal-derived H_2