Finding the Signal In the Noise

Determining North America's best path forward for sustainable energy

Canadian Journal of Chemical Engineering Lectureship Award Series

Thomas A. Adams II

Associate Professor, PhD, P.Eng
McMaster University
Department of Chemical Engineering
McMaster Advanced Control Consortium

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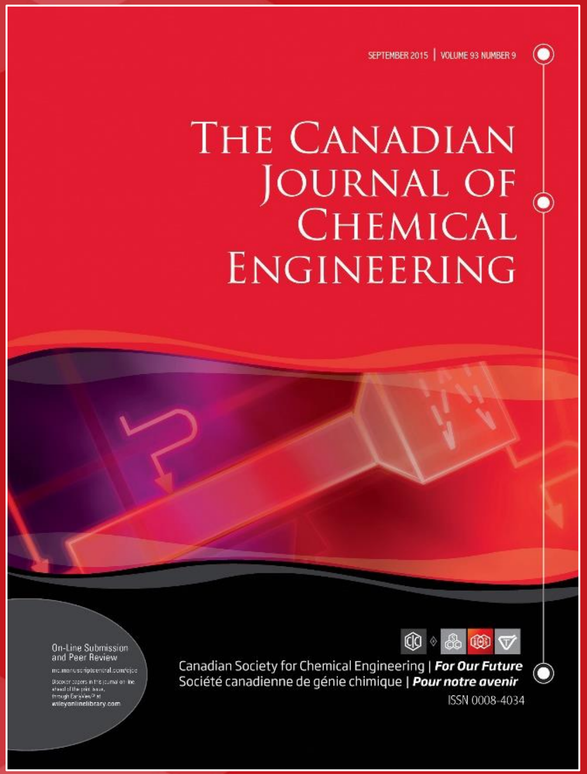

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Nease J, Adams TA II. Life Cycle Analyses of Bulk-Scale Solid Oxide Fuel Cell Power Plants and Comparisons to the Natural Gas Combined Cycle. *Canadian J Chem Eng*, 93:1349-1363 (2015).
(and others)

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- Links to articles cited in the study
- Links to data sets and simulations used in cited studies

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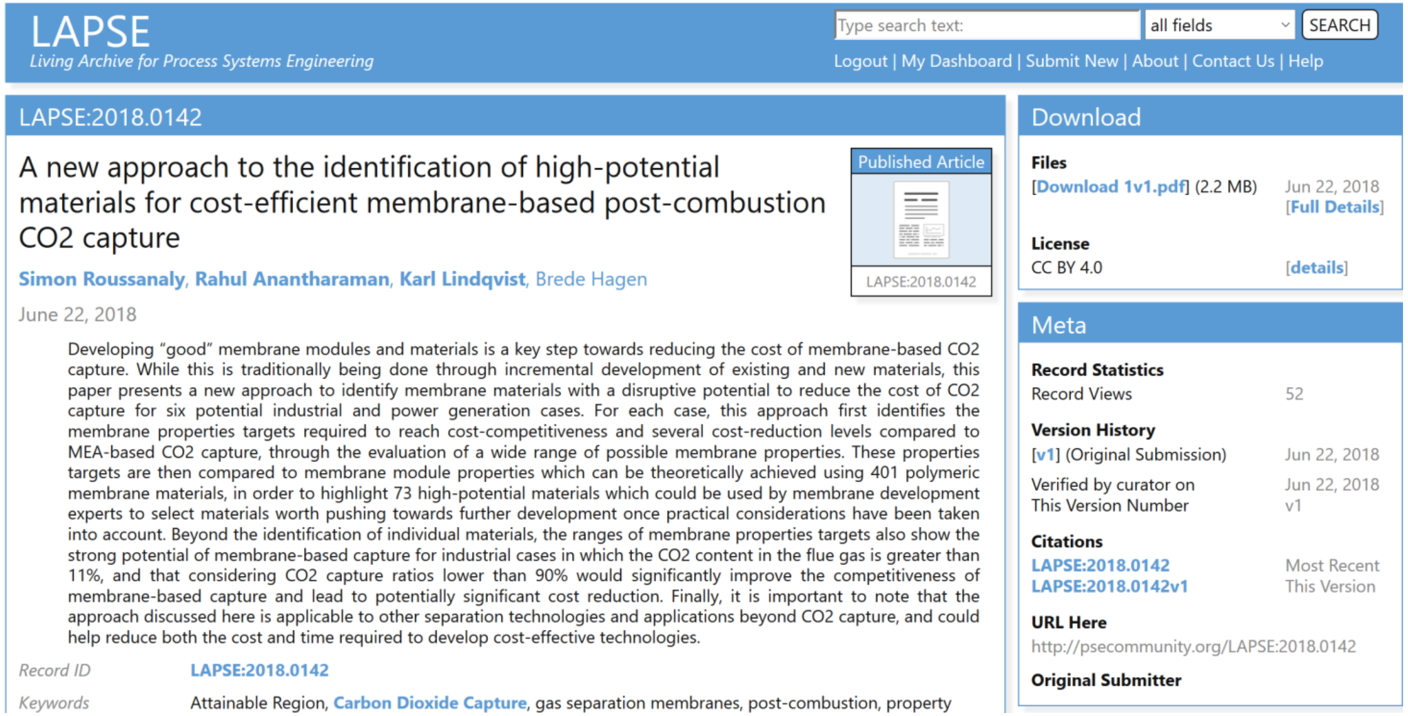

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LAPSE:2018.0142

A new approach to the identification of high-potential materials for cost-efficient membrane-based post-combustion CO2 capture

Published Article
LAPSE:2018.0142

Simon Roussanaly, **Rahul Anantharaman**, **Karl Lindqvist**, Brede Hagen

June 22, 2018

Developing "good" membrane modules and materials is a key step towards reducing the cost of membrane-based CO2 capture. While this is traditionally being done through incremental development of existing and new materials, this paper presents a new approach to identify membrane materials with a disruptive potential to reduce the cost of CO2 capture for six potential industrial and power generation cases. For each case, this approach first identifies the membrane properties targets required to reach cost-competitiveness and several cost-reduction levels compared to MEA-based CO2 capture, through the evaluation of a wide range of possible membrane properties. These properties targets are then compared to membrane module properties which can be theoretically achieved using 401 polymeric membrane materials, in order to highlight 73 high-potential materials which could be used by membrane development experts to select materials worth pushing towards further development once practical considerations have been taken into account. Beyond the identification of individual materials, the ranges of membrane properties targets also show the strong potential of membrane-based capture for industrial cases in which the CO2 content in the flue gas is greater than 11%, and that considering CO2 capture ratios lower than 90% would significantly improve the competitiveness of membrane-based capture and lead to potentially significant cost reduction. Finally, it is important to note that the approach discussed here is applicable to other separation technologies and applications beyond CO2 capture, and could help reduce both the cost and time required to develop cost-effective technologies.

Record ID **LAPSE:2018.0142**

Keywords Attainable Region, **Carbon Dioxide Capture**, gas separation membranes, post-combustion, property

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Original Submitter

McMaster University ENGINEERING
MACC McMaster Advanced Control Consortium

Student Contribution Acknowledgements

Jake Nease
Professor at McMaster University
(Former PhD Student)

Leila Hoseinzade
Engineer at ArcellorMittal Dofasco
(Former PhD Student)

Pranav Madabhushi
PhD Candidate

Ikenna Okeke
PhD Candidate

Triple Bottom Line of Sustainability

Economical

- Capital
- Operating
- Supply Chain & Materials
- Job Creation / Losses
- Profitability
- Loans/Financing
- Stockholders
- Uncertainty and Risk

Environmental

- **Greenhouse Gases**
- **Particulates**
- **Deforestation**
- **Land Use / Transformation**
- **Resource Depletion**
- **Water Consumption**
- **Toxicity**
- **Wildlife Impact**
- **Noise**

Societal

- Public Acceptance
- NIMBYs
- BANANAs
- Health Impacts
- Public/Employee Safety
- Accidents
- Public Policy
- Electoral Politics

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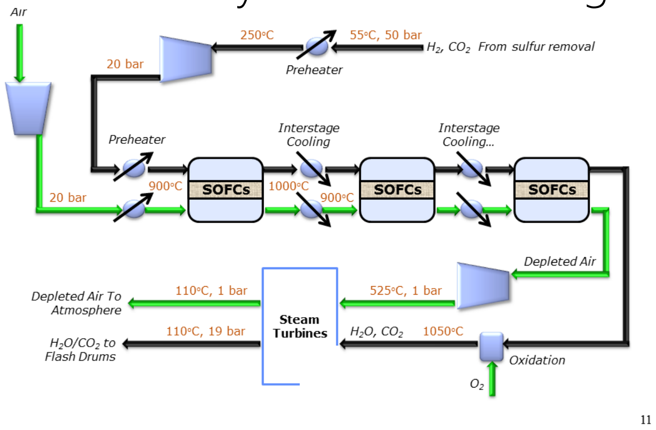
Sources: Jimenez-Gonzales and Constable. *Green Chemistry and Engineering, 2012. And contributions from many individuals.*

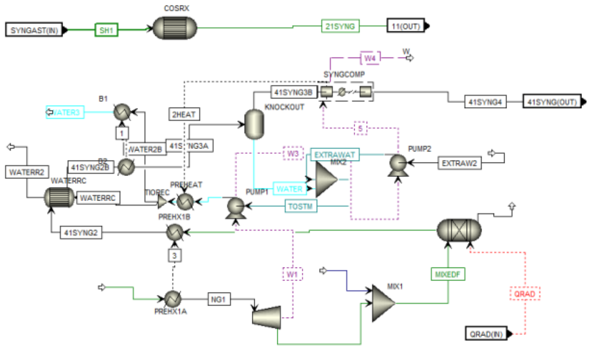
Big Picture – Adams Group Research Methods

Unit Operation Design

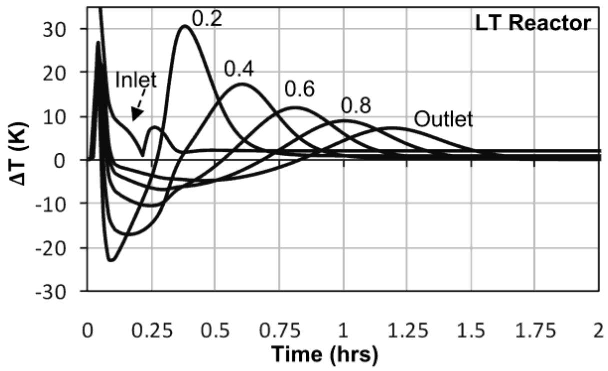
Process Synthesis and Design



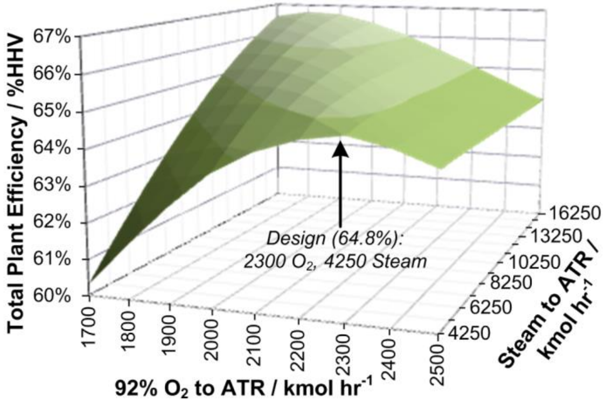
Process Modeling and Simulations



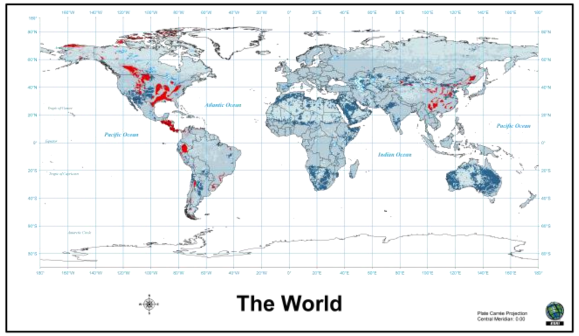
Process Dynamics



Process Optimization



Economics, Policy, and Environment (LCA)



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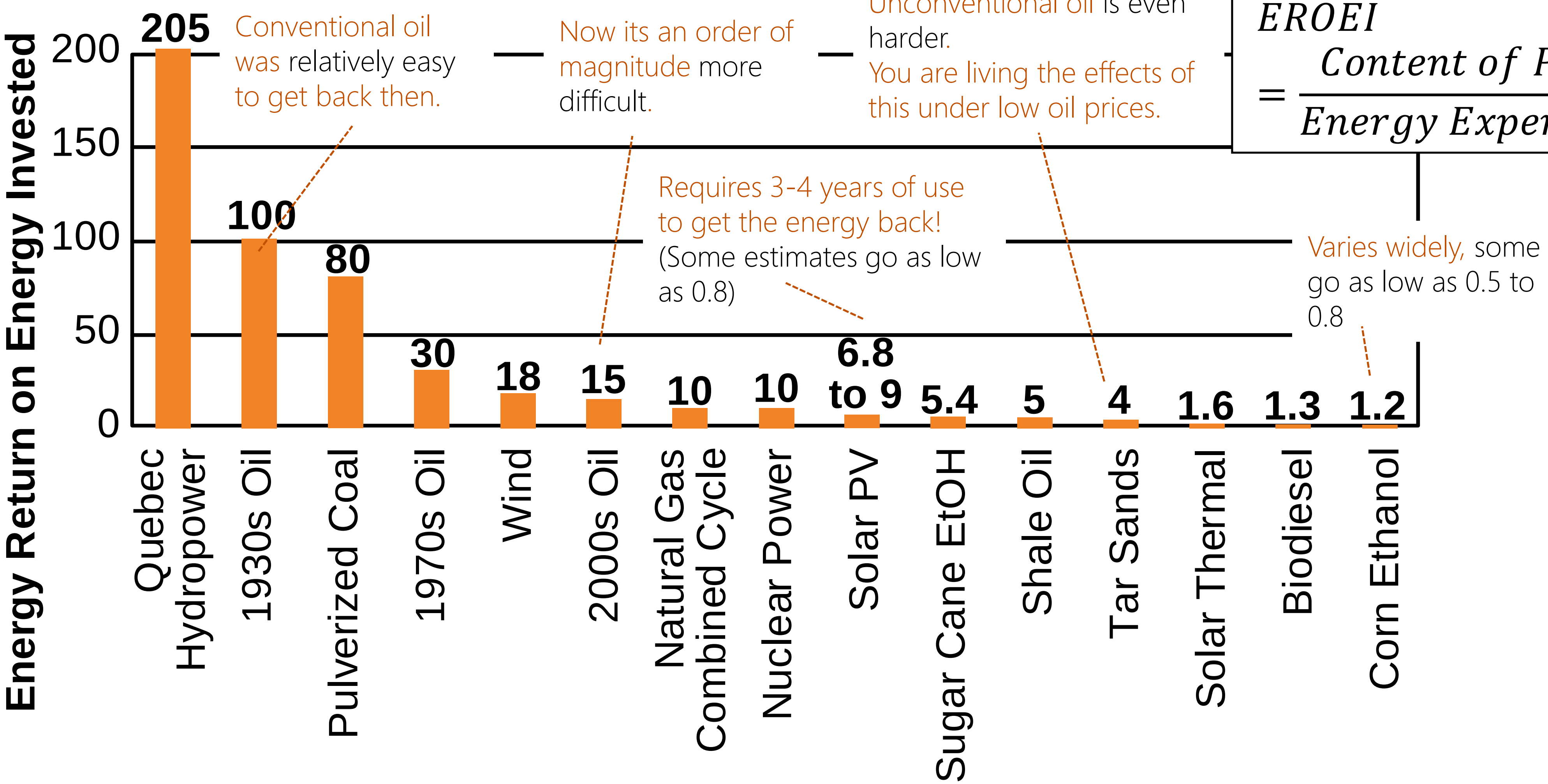
Energy Return on Energy Invested (EROEI)

$$EROEI = \frac{Content\ of\ Product\ Delivered}{Energy\ Expended\ To\ Produce\ It}$$



Sources: A. Poisson, C.A.S. Hall, 2013. Time series EROI for Canadian oil and gas. *Energies*, 6, 5940-5959.
A.K. Gupta, C.A.S. Hall, 2011. A review of the past and current state of EROI data. *Sustainability*, 3, 1796-1809.
D.J.R. Murphy and C.A.S. Hall, 2010, Year in review—EROI or energy return on (energy) invested. *Ann NY Acad Sci*, 1185,102-118.
Raugei M et al. 2017. *Energy Policy* 102:377-384. Ferroni, Guekos, and Hopkirk, 2017, *Energy Policy* 107:498-505.

Disclaimer: This is an overly simplistic metric with wide variability depending on data, assumptions and methods. But it's still useful to make my point.

Scale and Why It Matters

- At \$50/tonne CO_2 emission tax (Canada Federal 2022 Minimum)
  - Global CO_2 Emissions: 36 billion tonne / yr
  - Global Tax Value: \$1.8 trillion / year (2.4% of World GDP)
  - Canada's GDP: \$1.5 trillion / year
- This is how the three tiers are linked in practice for Canada
  - (For climate change at least)
- Key Tools for Chemical Engineers:
  - Techno-economic analysis (TEA)
  - Life cycle analysis (LCA)

Sources: Environment and Climate Change Canada. *Pricing carbon pollution in Canada: how it will work*. Accessed October 2017.
PBL Netherlands Environmental Assessment Agency. *Trends in Global CO2 Emissions*, 2016.
The World Bank Databank, *GDP (Current USD)*, Accessed Oct 2017.

Big Picture Motivation

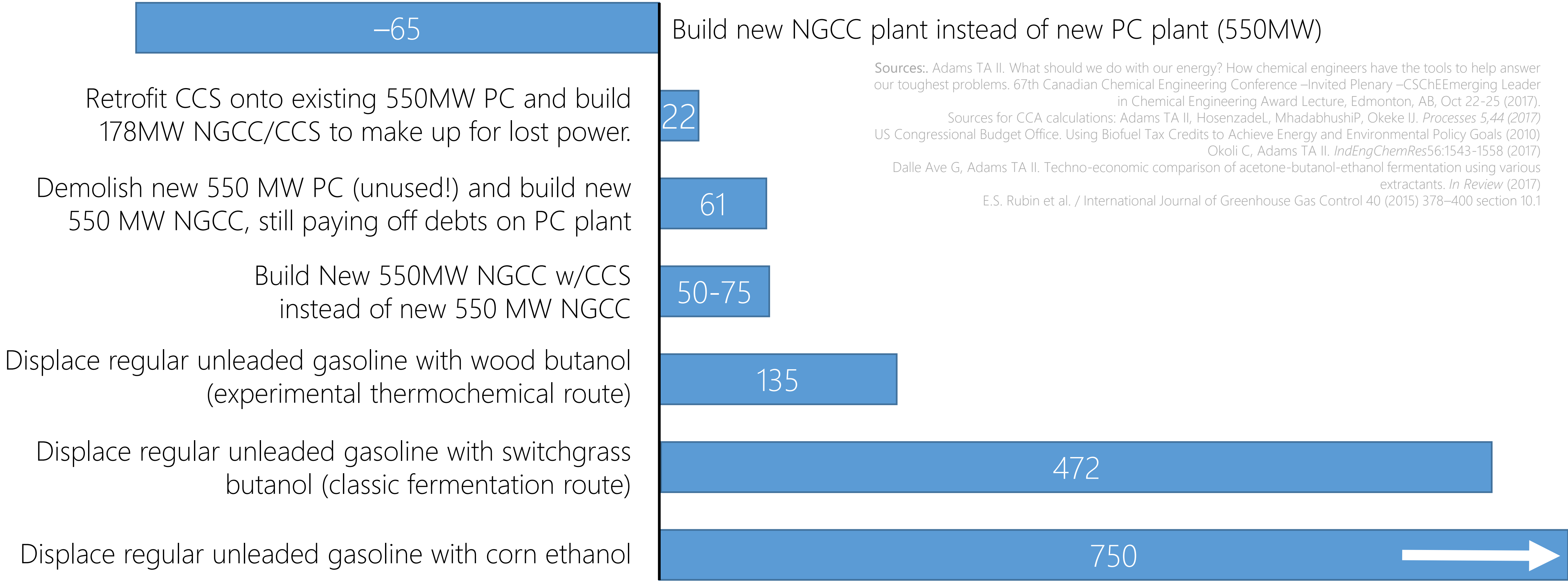
- We have so many technology ideas for reducing greenhouse emissions.
- Which should we focus on now?
- Where should our money be invested?
- What should we do first, and then next?

Cost of CO_2 Avoided: Where do we invest $$$?

$$CCA = \frac{Cost\ of\ Option\ 2\ - Cost\ of\ Status\ Quo}{GHG\ Emissions\ of\ Status\ Quo\ - GHG\ Emissions\ of\ Option\ 2}$$

- Both should yield same product/service
- Use Life Cycle emissions

CCA (in 2016$US per tonne of CO_2 equivalents)

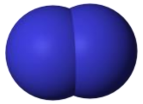
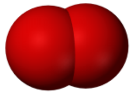
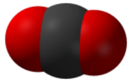


Sources:. Adams TA II. What should we do with our energy? How chemical engineers have the tools to help answer our toughest problems. 67th Canadian Chemical Engineering Conference –Invited Plenary –CSChEEmerging Leader in Chemical Engineering Award Lecture, Edmonton, AB, Oct 22-25 (2017).
Sources for CCA calculations: Adams TA II, HosenzadeL, MhadabhushiP, Okeke IJ. *Processes 5,44 (2017)*
US Congressional Budget Office. Using Biofuel Tax Credits to Achieve Energy and Environmental Policy Goals (2010)
Okoli C, Adams TA II. *IndEngChemRes*56:1543-1558 (2017)
Dalle Ave G, Adams TA II. Techno-economic comparison of acetone-butanol-ethanol fermentation using various extractants. *In Review* (2017)
E.S. Rubin et al. / International Journal of Greenhouse Gas Control 40 (2015) 378–400 section 10.1

Fundamental Problem of CO_2 Capture and Sequestration

- **Fundamental problem**: separation of CO_2 and N_2 in flue gases:
  - We need to go from dilute to high purity
- We need to go from low pressure to high pressure
- And there's an awful lot of it (~7 million ton/yr per coal power plant).

TYPICAL COAL POWER FLUE EXHAUST, 1 BAR

	Mol %	Kinetic Diameter (Images to Scale)	
N_2 (&Ar)	68%		3.6 Å
O_2	2%		3.45 Å
CO_2	13%		3.30 Å
H_2O	17%		2.7 Å

CO_2 PIPELINE LIMITS, 120 BAR

	Kinder Morgan	Sleipner
N_2 (&Ar)	<4%	3-5%
O_2	<50ppm	<50ppm
CO_2	>95%	93-96%
H_2O	<690ppm	<Saturated

Sources: NETL 2007 - Bituminous Baseline Report (see required reading). Adams & Barton, AIChE J (2010)
deVisser E., et al. Dynamis CO2 quality recommendations. Int. J. Greenhouse Gas Cont. 2008, 2, 478–484
Molecule Images from chemistry.about.com. Sizes from Angew. Chem. Int. Ed. 2010, 49, 6058 – 6082.

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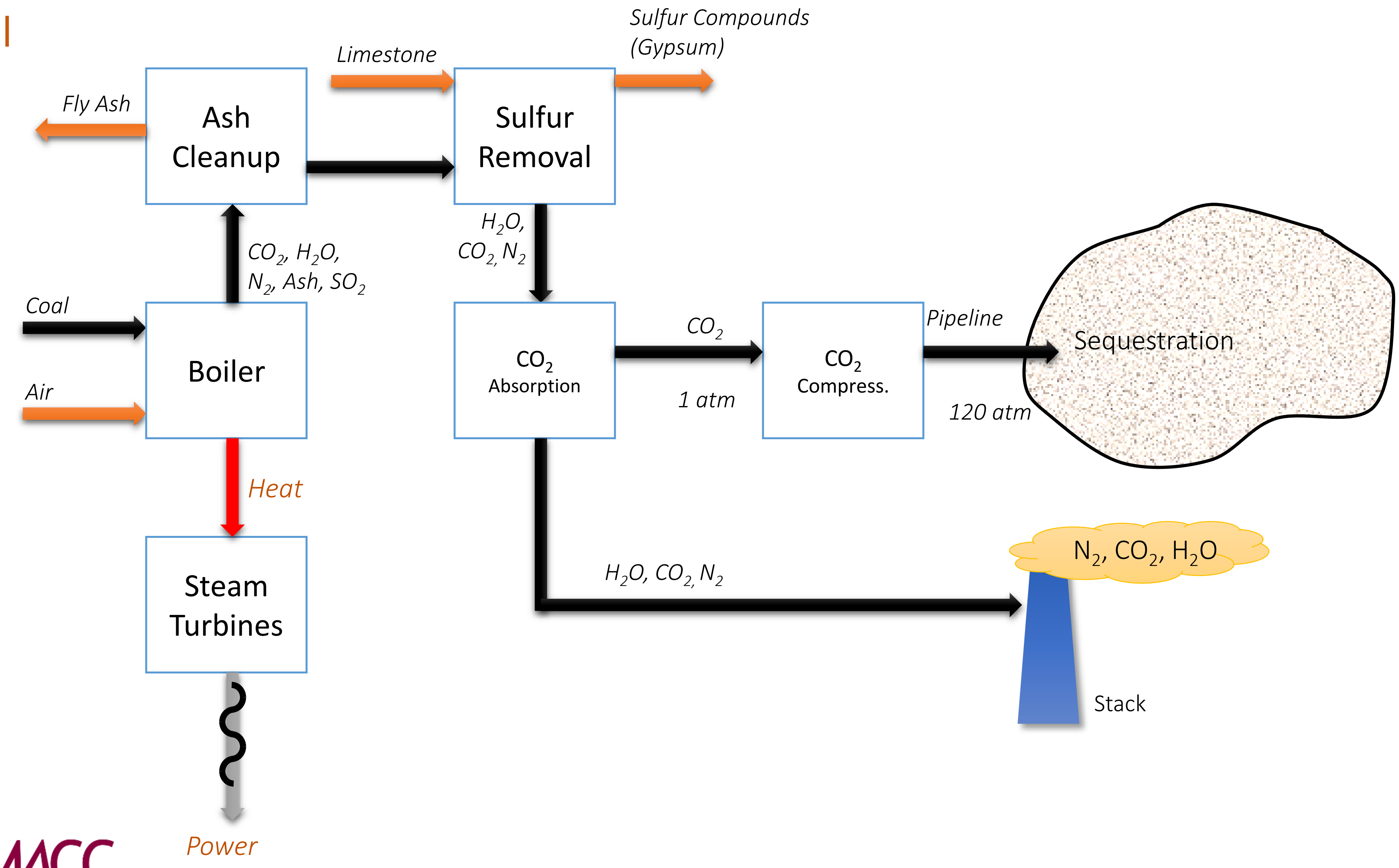
Post-Combustion Solvent-Based Capture

Pulverized Coal Example

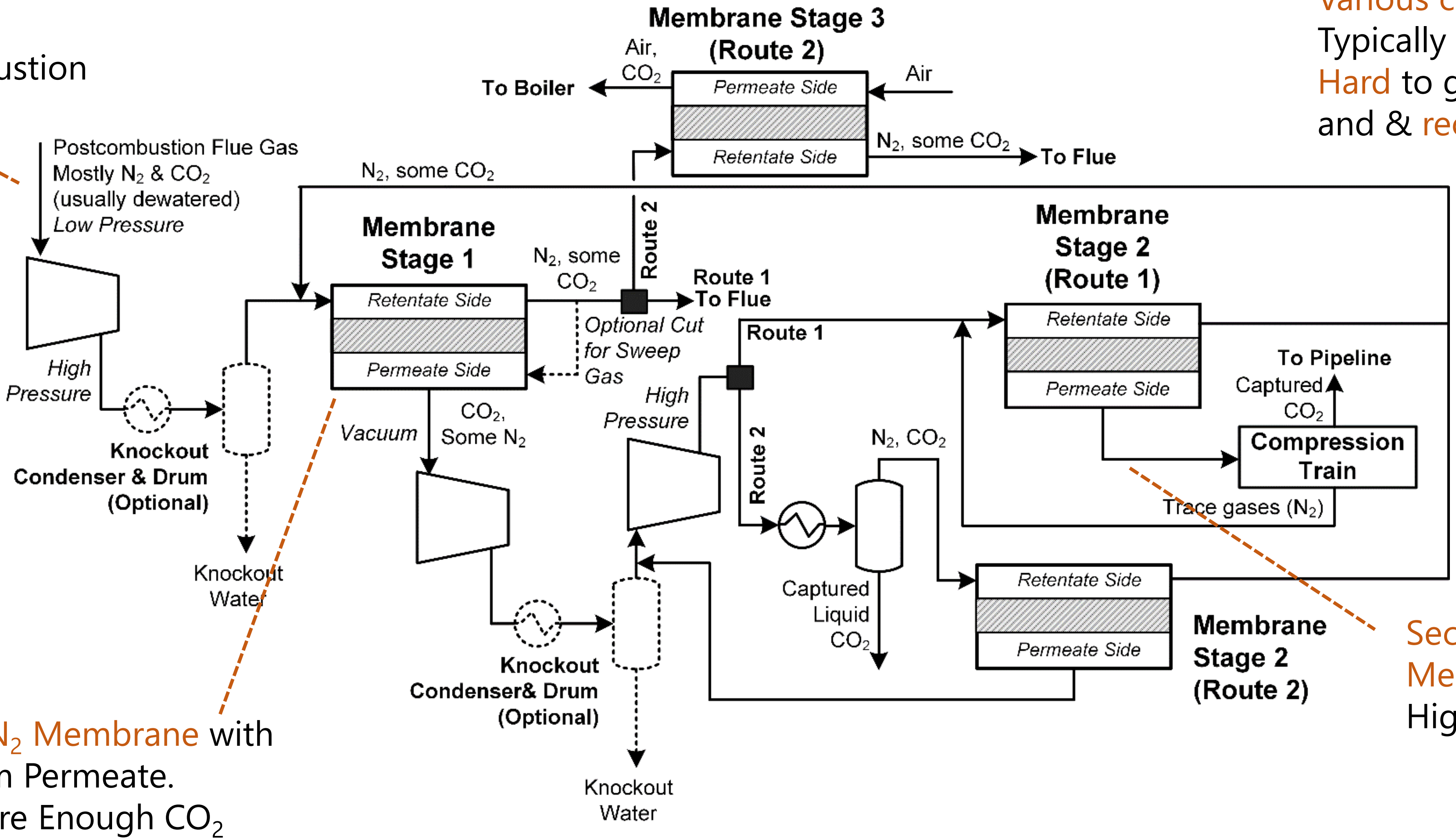


Source: NETL 2007 - Bituminous Baseline

Post-Combustion Membrane-Based Capture

Flue Gas from
Upstream Combustion

Various configurations
Typically 2 or 3 stages
Hard to get both purity and & recovery



CO_2 / N_2 Membrane with Vacuum Permeate.
Not Pure Enough CO_2

Second CO_2 / N_2 Membrane
Higher Purity CO_2

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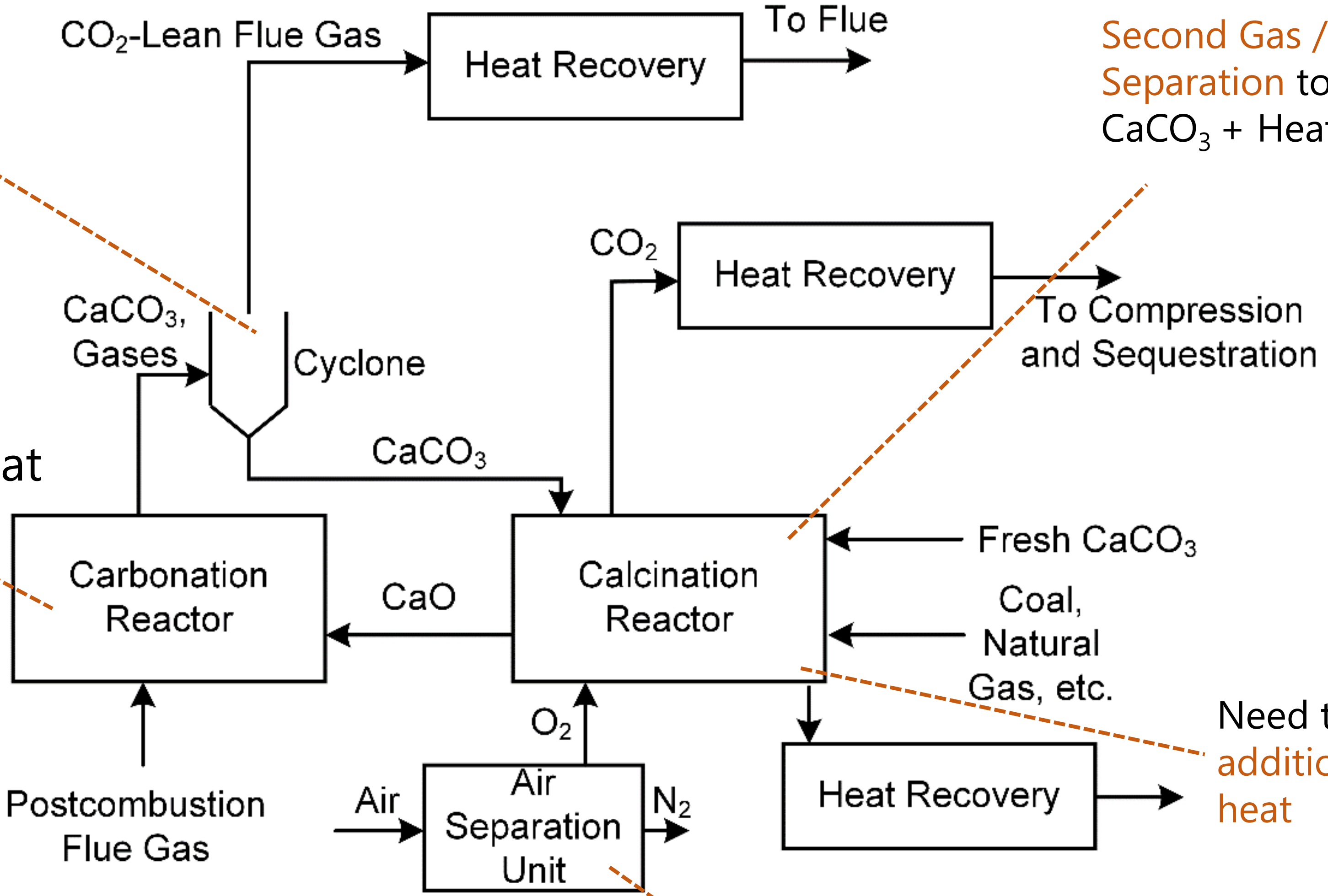
Source: Adams TA II, Hoseinzade L, Madabhushi P, Okeke IJ. Processes 5:44 (2017).

Post-Combustion Solid-Based Capture

Solid Calcium Carbonate Cycloned from rest of flue gases

Second Gas / Solid Separation to release CO_2.
$CaCO_3 + Heat \rightarrow CaO + CO_2$

$CaO + CO_2 \rightarrow CaCO_3 + Heat$



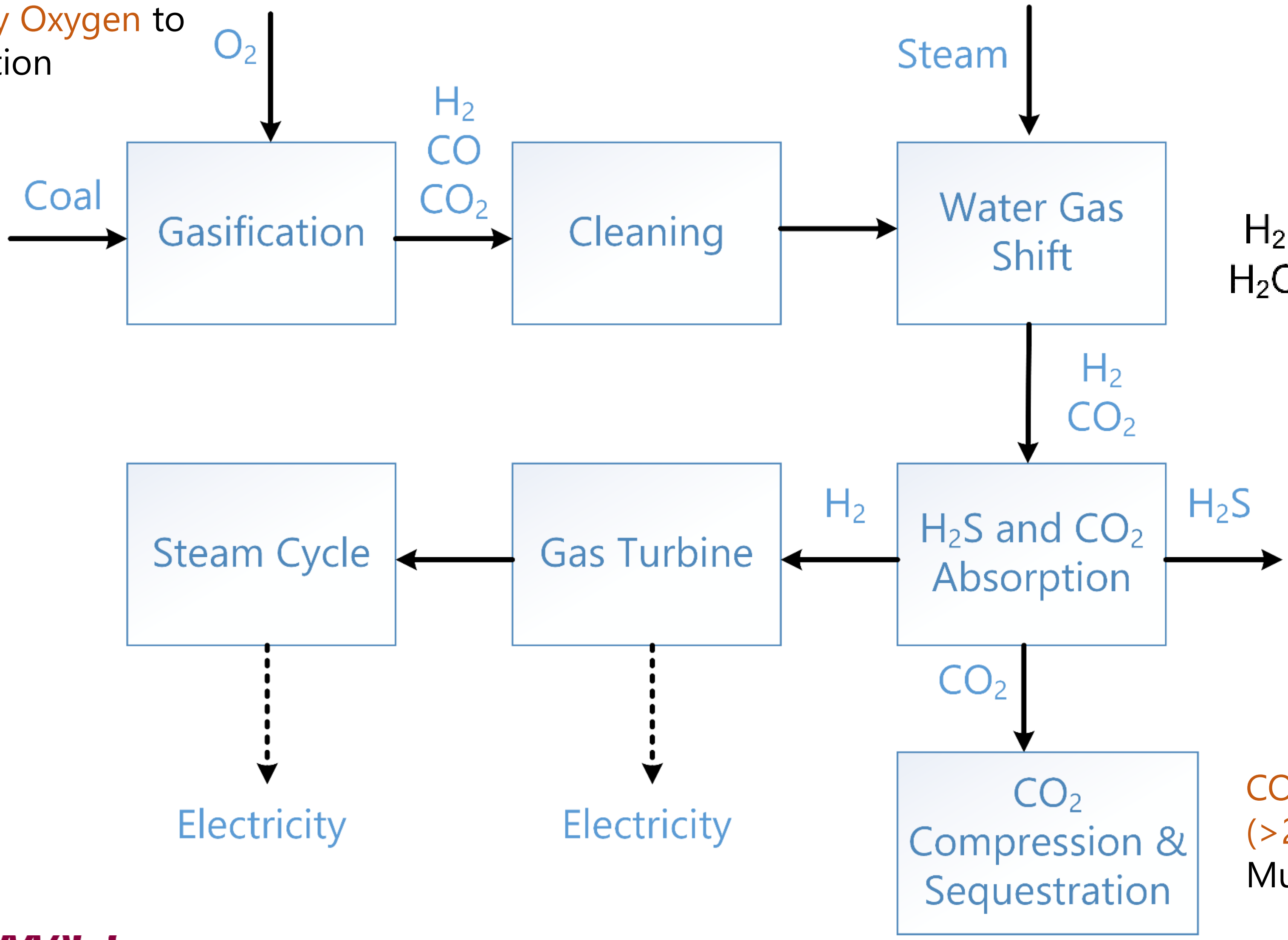
Need to **burn additional fuel for heat**

Need High Purity Oxygen to prevent N_2 injection

Source: Adams TA II, Hoseinzade L, Madabhushi P, Okeke IJ. Processes 5:44 (2017).

Pre-Combustion Solvent-Based Capture (IGCC)

Need High Purity Oxygen to prevent N_2 injection



WGS Reactors

$H_2O + CO \rightarrow CO_2 + H_2$

$H_2O + COS \rightarrow CO_2 + H_2S$

Selexol or Rectisol Solvents

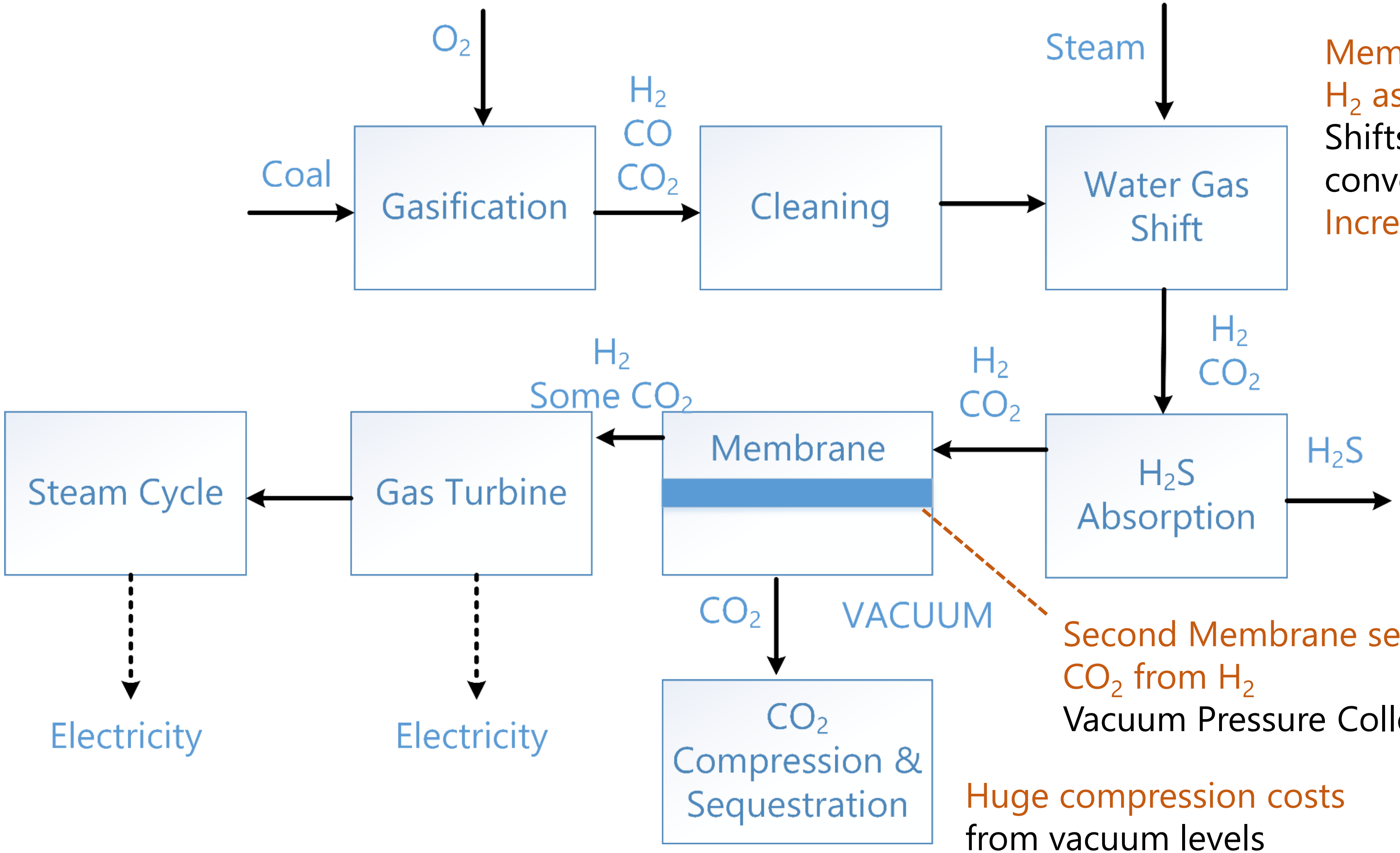
Capture H_2S and CO_2 in separate stages

H_2/CO_2 Separation Principle

CO_2 captured at higher pressures (>20 bar)

Much lower compression costs

Pre-Combustion Membrane-Based Capture



Membrane-enhanced WGS removes H_2 as produced

Shifts equilibrium to toward higher conversion

Increases CO_2 concentration for later

Second Membrane separates CO_2 from H_2

Vacuum Pressure Collection

Huge compression costs from vacuum levels

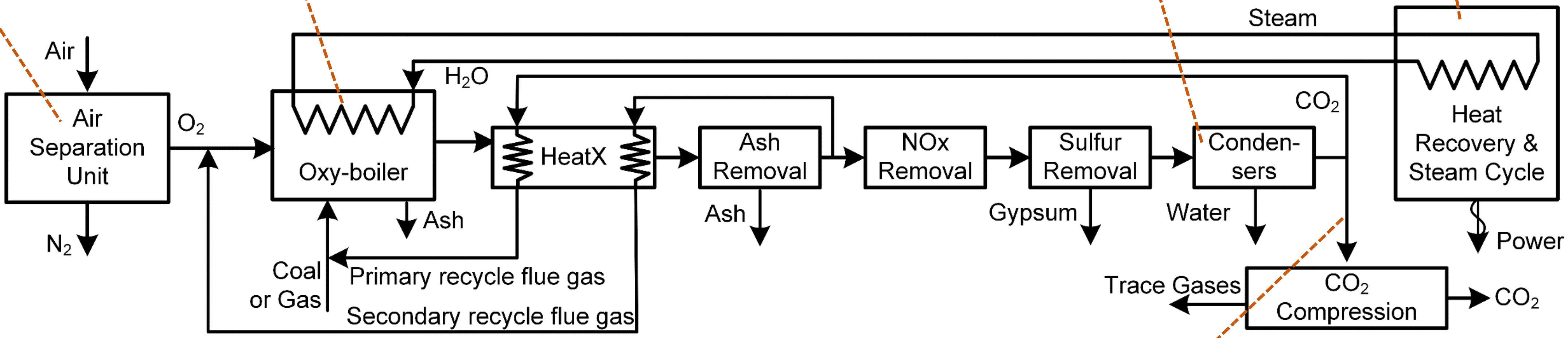
Oxyfuel Combustion

Fuel combusted in N2-free flame
Diluted with CO_2 for thermal management

Very Large ASU

CO_2/H_2O Separation
via water condensation

Power Produced through
Steam Cycles



CO2 captured at
atmospheric pressure

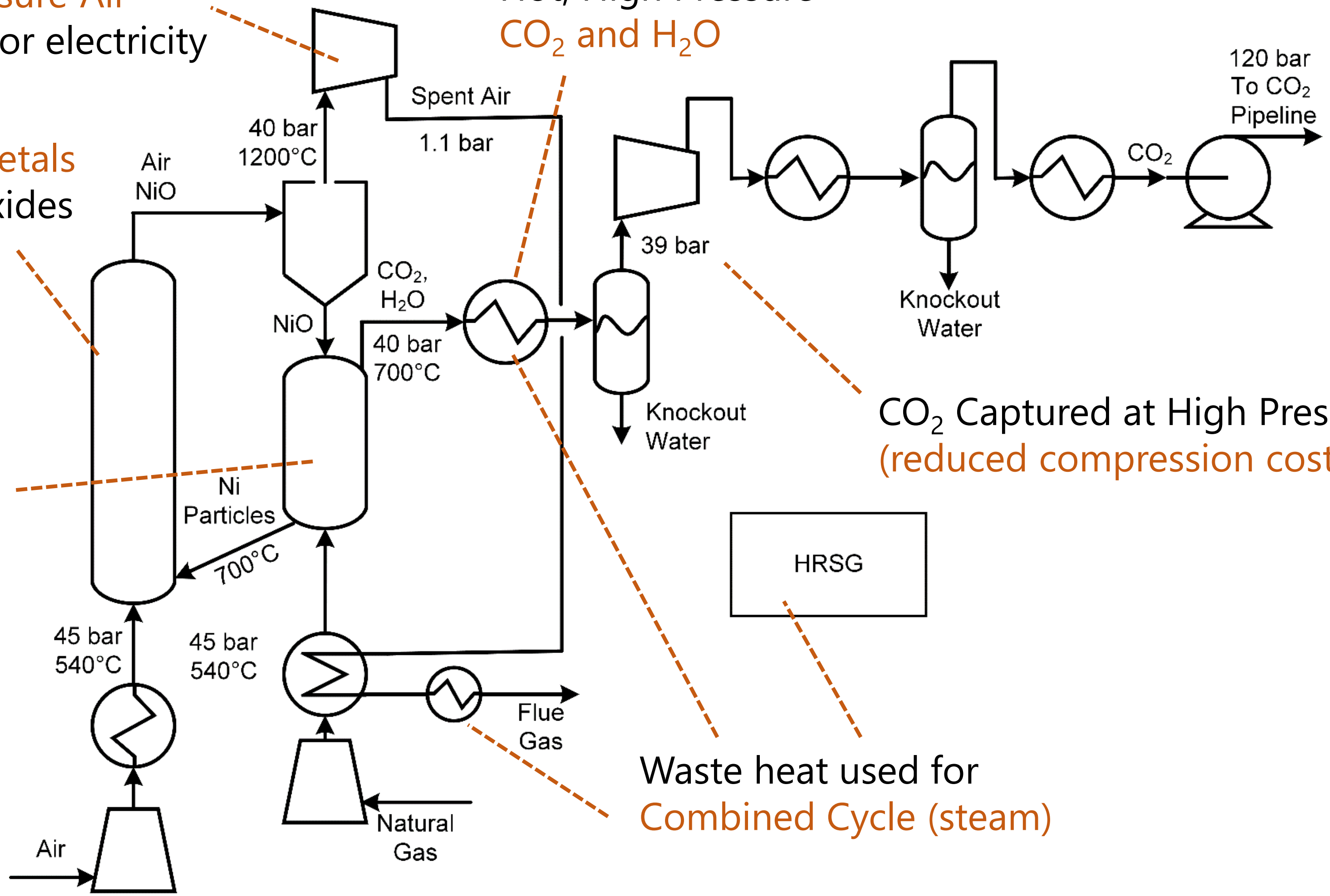
Chemical Looping Combustion

Hot, High Pressure Air
Spins turbine for electricity

Hot, High Pressure
CO_2 and H_2O

Air reacts with reduced metals
Creates heat and metal oxides
$O_2 + Me \rightarrow MeO + Heat$

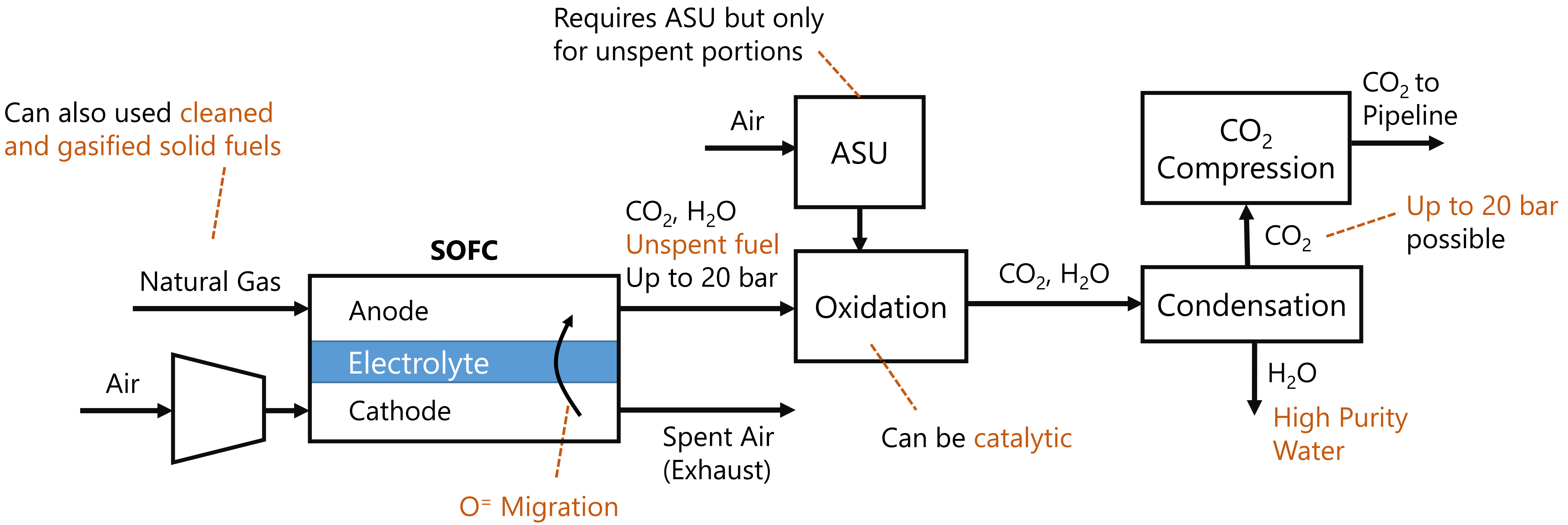
Fuel combusts using
metal oxides instead of air
$MeO + CH_4 + Heat \rightarrow$
$H_2O + CO_2 + Me$



CO_2 Captured at High Pressure
(reduced compression costs)

Waste heat used for
Combined Cycle (steam)

Solid Oxide Fuel Cell (SOFC) Process



Recap

Type	Separation Problem	ASU Requirements	CO_2 Capture Pressure	Example Applications
Solvent-based Post-Combustion	CO_2/N_2	—	1 bar	Pulverized Coal, NGCC
Membrane-Based Post-Combustion	CO_2/N_2	—	Vacuum	Pulverized Coal, NGCC
Solid-Based Post-Combustion	CO_2/N_2	Low	1 bar	Pulverized Coal, NGCC
Solvent-Based Pre-Combustion	CO_2/H_2	Medium	10-50 bar	IGCC, pre-reforming NGCC
Membrane-Based Pre-Combustion	CO_2/H_2	Medium	Vacuum	IGCC, pre-reforming NGCC
Oxyfuels	CO_2/H_2O	High	1 bar	Gasified Coal/Nat Gas
Chemical Looping	CO_2/H_2O	—	10-50 bar	Gasified Coal/Nat Gas
Solid Oxide Fuel Cells	CO_2/H_2O	Low	1-20 bar	Gasified Coal/Nat Gas

Key Problems

- No systematic comparison between processes
- Everyone claims their own process is the best when compared against some other
- Wide variation in assumptions, strategies and ideas.

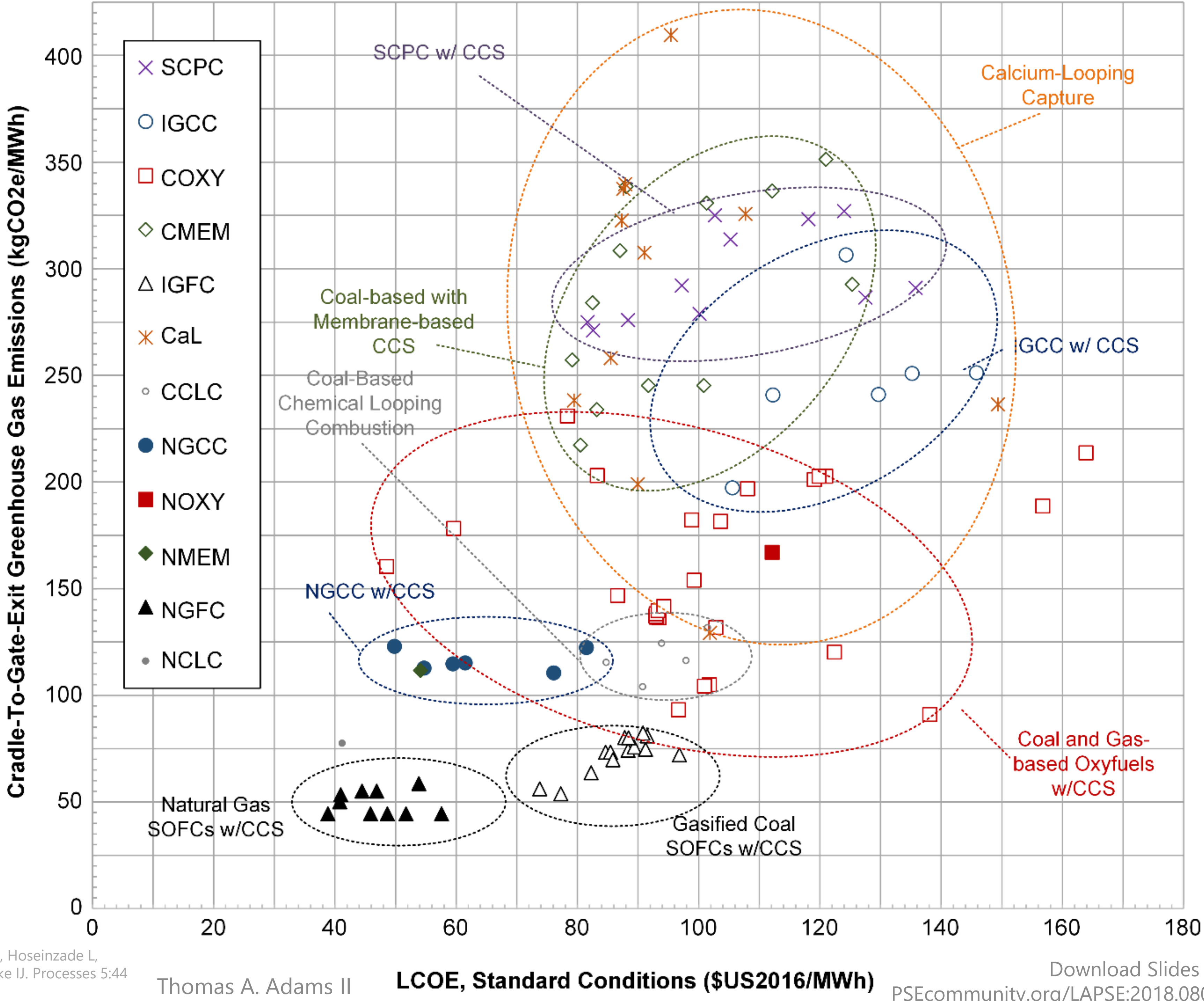
- Solution: Meta-Study of ~100 published data points on those 8 processes.
- Convert to a standard basis of comparison

Standards

- Size: 550 MW net, plant gate
  - Nonfuel costs scaled with power law method p=0.9
- Time & Place: 1Q2016 USA
  - Time: North American Plant Cost Index
  - Place: Purchasing Power Parity Index
- Fuel
  - US Bituminous Coal #6 2016 Avg Price
  - US Conventional Average Gas Mix 2016 Avg Price
- Captured CO_2 at plant gate
  - Pressure: >115 bar
  - Purity: >95 mol%
  - Capture Rate: 90-100%
- LCA: Cradle to Gate GHG
  - Consistent NOx production where neglected in original
  - Standardize cradle-to-plant-entrance life cycle impacts
- CCA: Cost of CO_2 Avoided
  - Same standard plant without CCS
  - SCPC and NGCC US baseline std's

Overall

- SOFC clear winner for coal and gas
- NGCC w/CCS excellent near term solution
- No point in using membranes!
- Oxyfuels / CLC good coal intermediate step



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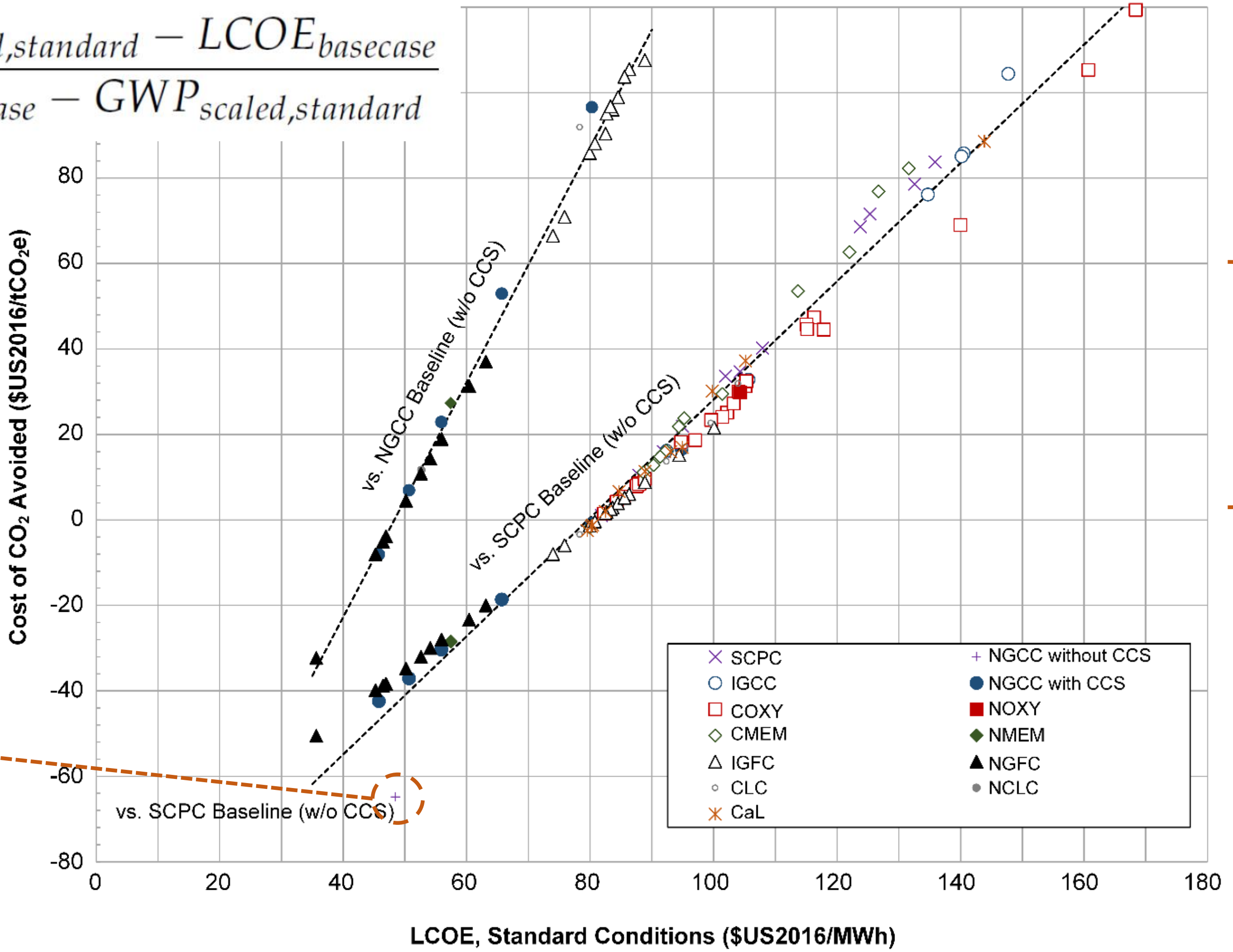
Source: Adams TA II, Hoseinzade L, Madabhushi P, Okeke IJ. Processes 5:44 (2017).

Cost of CO_2 Avoided

$$CCA = \frac{LCOE_{scaled,standard} - LCOE_{basecase}}{GWP_{basecase} - GWP_{scaled,standard}}$$



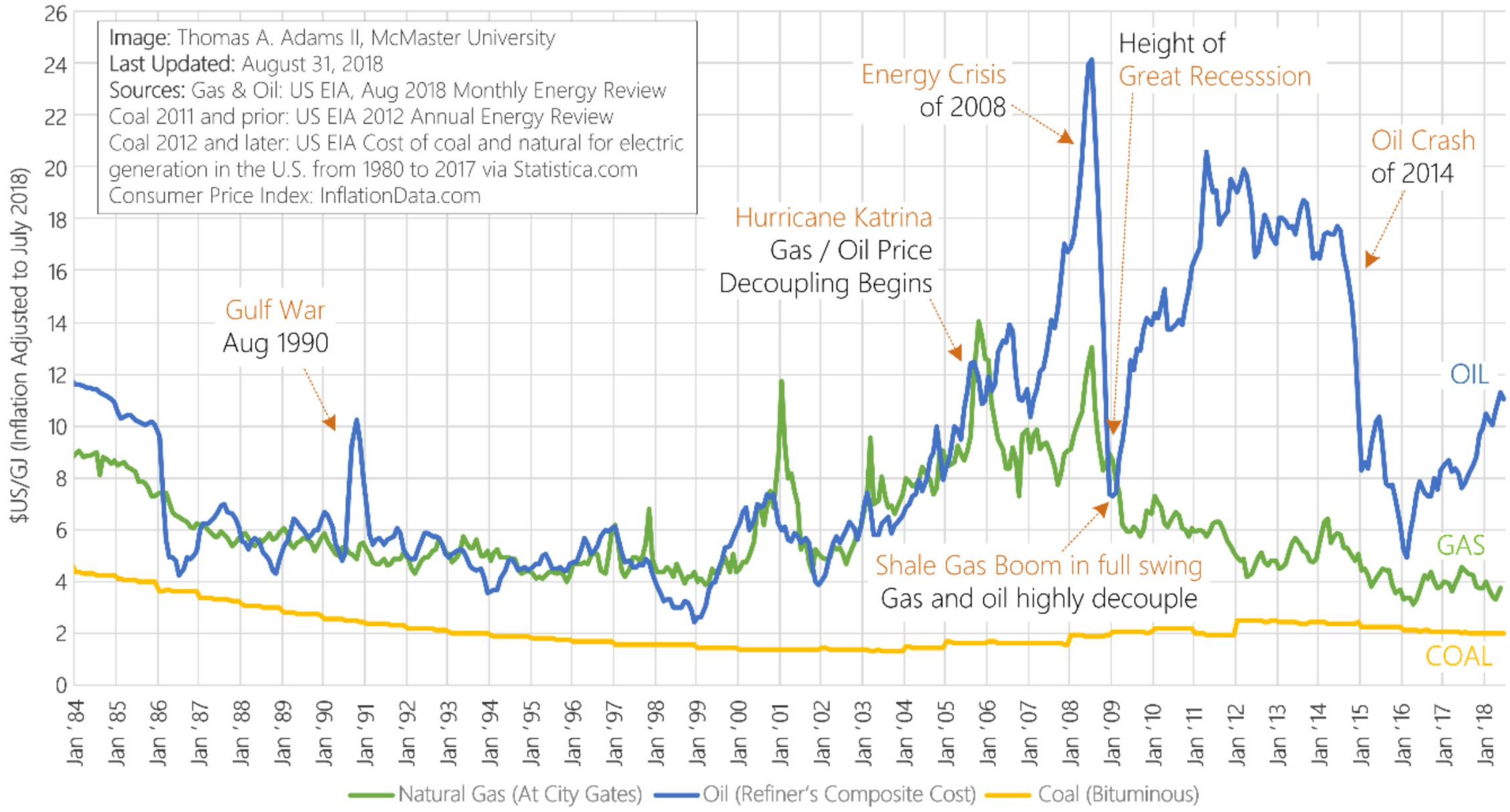
Special Point:
Switching from coal to gas w/o CCS
No point to new coal at all in North America!

Sweet Spot:
The best of post-combustion solvent systems are the only mature technology to be competitive.
Rest requires CO_2/H_2O style power gen.

Negative CCA means:
Gas is so cheap in North America, there is no point to using coal at all.

Source: Adams TA II, Hoseinzade L, Madabhushi P, Okeke IJ. Processes 5:44 (2017).

Price Trends



Meta-Study Conclusions

- No point to building new coal
  - (as long as gas prices stay low)
  - IGCC cannot compete with SCPC
  - Calcium Looping unlikely to either
- Membranes not so promising
  - Coal: Only fictional membranes could compete with solvents at the system level
  - Gas: At best competes with solvent directly, maturity / lifetime issues aside.
- SOFC is best way to use coal
  - (Could be better than gas in Asian context. Asian study needed!)

FINAL RECOMMENDATIONS

- Near Term: Use NGCC with CCS
  - Closest thing we have to commercial
- Long Term: Use SOFCs with CCS
  - Needs research and investment now
  - Best fossil fuel approach possible
  - Translates well in foreign situations

Expanding and Standardizing

Big Picture Lessons from Study

- Rather hard to do cross-comparative research of eco-techno-economic analyses (ETEAs)
- But the rewards of doing meta-studies like this are significant
- A standardization of ETEA methodology for the field would greatly amply the impact of each of our own studies

~O(1,000-10,000) researcher-hours

Very useful society, business, and policy conclusions

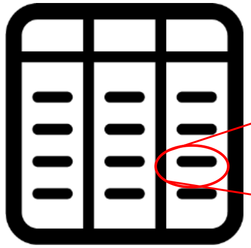
Individual studies would have greater influence

Proposal: Develop recognized standards for performing TEAs and ETEAs

Standard Types	Details….
Base Case Status Quo For Comparison	"Standard" power plants, "standard" refineries, "standard" chemical processes, etc.
Life Cycle Analysis Methodologies	Existing ISO standards, boundary definitions, impact analyses assumptions, methods, etc.
Plant Sizing / Delivered Products	Standard representative capacities and qualities
Metric Definitions	CCA, NPV, efficiencies, HHV vs LHV, other assumptions
Cost Estimations	Standard cost curves, approaches, and assumptions
Transparency and Verifiability	Spreadsheets and models released open-access
Data Formats	Open document formats, etc.

Example Use of Standards: Authors

Researcher Defines ETEA Study as Usual



Consults standards table

PSE-3:
Fuels,
North America,
Large Scale

Selects appropriate, scenario, assumptions and metrics

Research Performed

$NPV_{PSE\text{-}3}$ = \$1.2 bln

$CCA_{PSE\text{-}3}$ = \$40.3/tonne

$GHG_{PSE\text{-}3}$ = 4.5 tCO_2e

Metrics Computed according to Standard

$NPV_{alternate}$ = \$1.3 bln

$CCA_{alternate}$ = \$41.3/tonne

$GHG_{alternate}$ = 4.2 tCO_2e

Non-standard metrics also reported (special cases, etc.)

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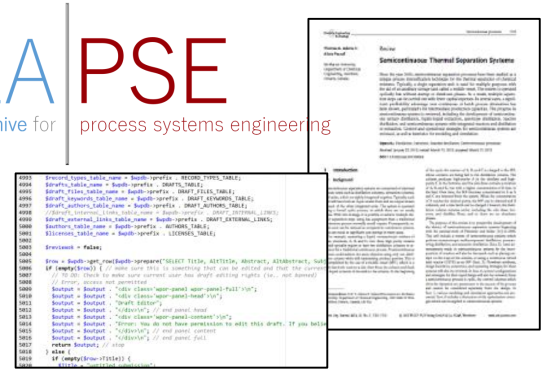

Paper Published. Models / spreadsheets / code released to public database

Example Use of Standards: Readers

Reader studies paper using PSE standard

$$NPV_{PSE\text{-}3} = \$1.2 \text{ bln}$$

$$CCA_{PSE\text{-}3} = \$40.3/\text{tonne}$$

$$GHG_{PSE\text{-}3} = 4.5 \text{ tCO}_2\text{e}$$

Reader sees standard metrics, immediately understood

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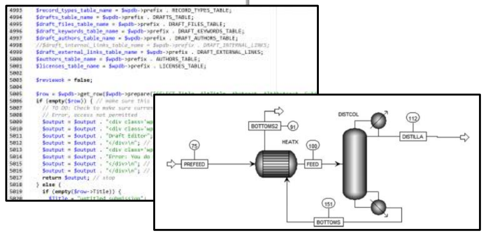
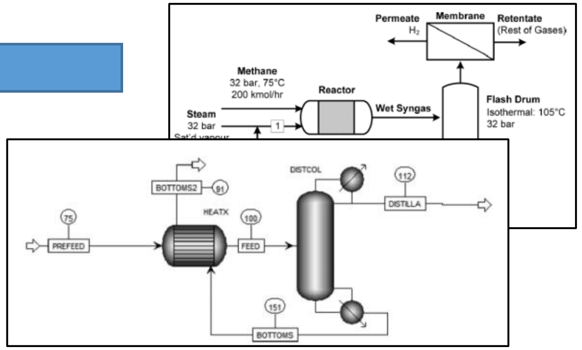


Reader downloads files and data to verify results

Reader considers other papers using the same standards



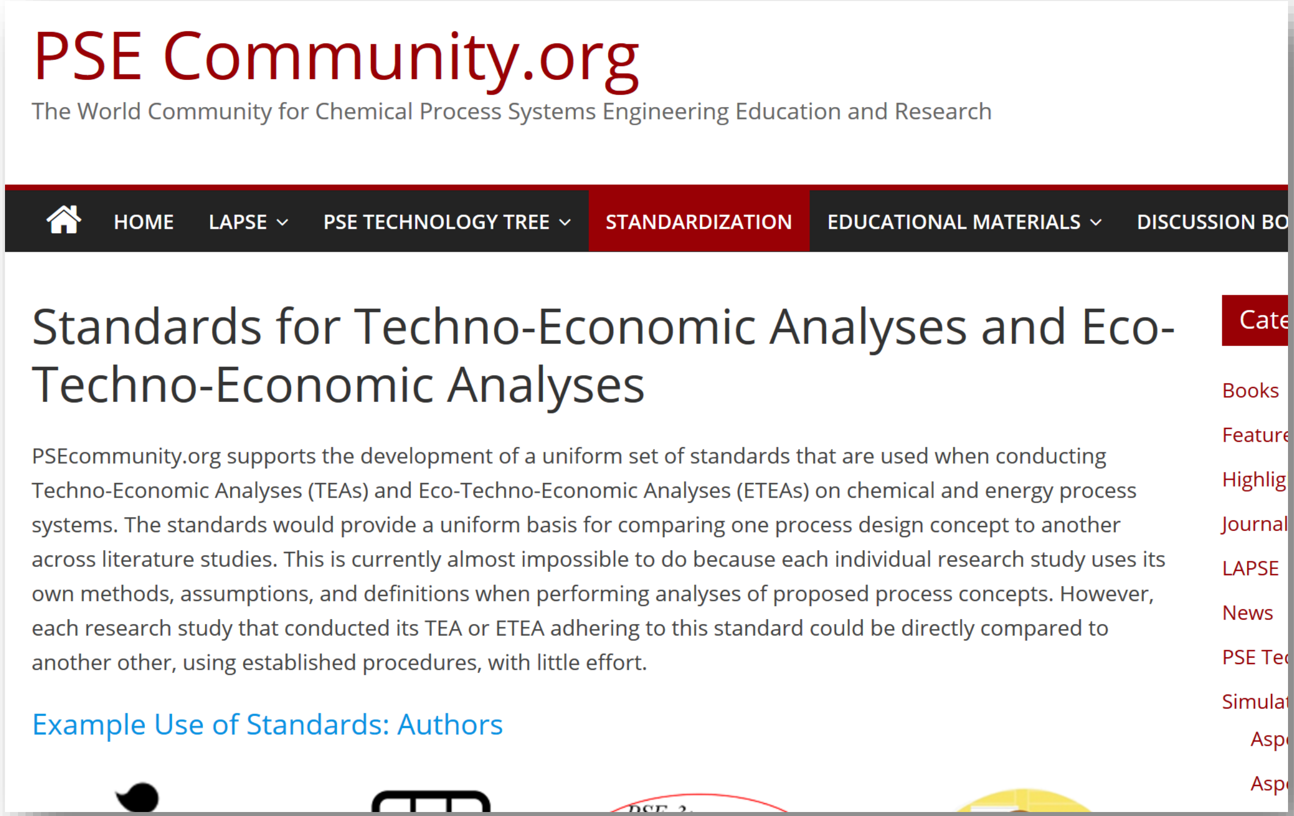
Reader easily incorporates standardized models into own work

Reader rapidly performs comparisons and research

All standardized research has high impact and citations!

Standardization Committee

- Call for members and stakeholder input
- Go to http://PSEcommunity.org/standards



Wrap Up

- We can learn a lot from eco-techno-economic meta studies
  - Critical for taking meaningful and near-term action on climate change
  - Critical for policy and business
  - See through the hype.
- Current culture of the field:
  - Hide models and code
  - C.Y.A.
  - Nonstandard methods
  - Not working toward common goal
- Goal: Make it as easy as possible for others to use and understand your research for societal benefit
  - Join me!