Maximizing Our Impact

A call for the standardization of techno-economic analyses for sustainable energy systems design research.

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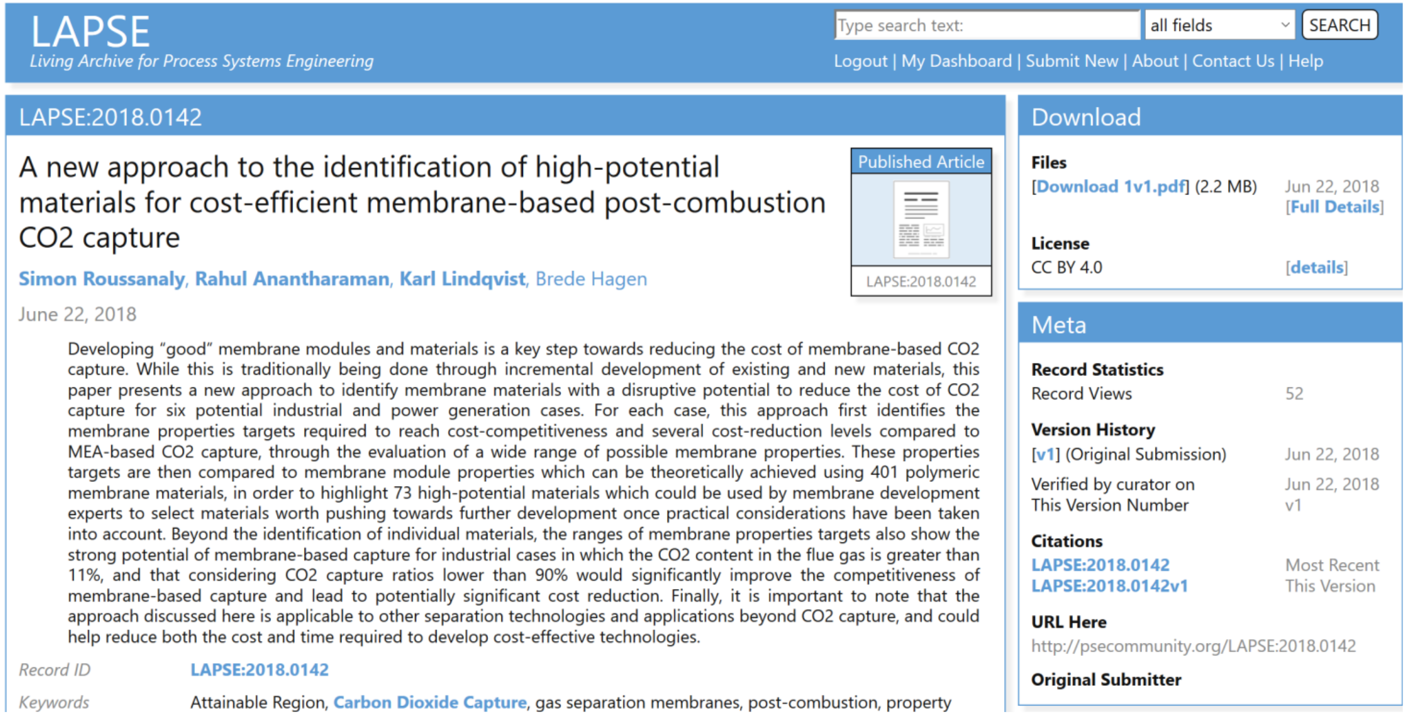
- Links to articles cited in the study
- Links to data sets and simulations used in cited studies



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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

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Triple Bottom Line of Sustainability

Economical

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

Environmental

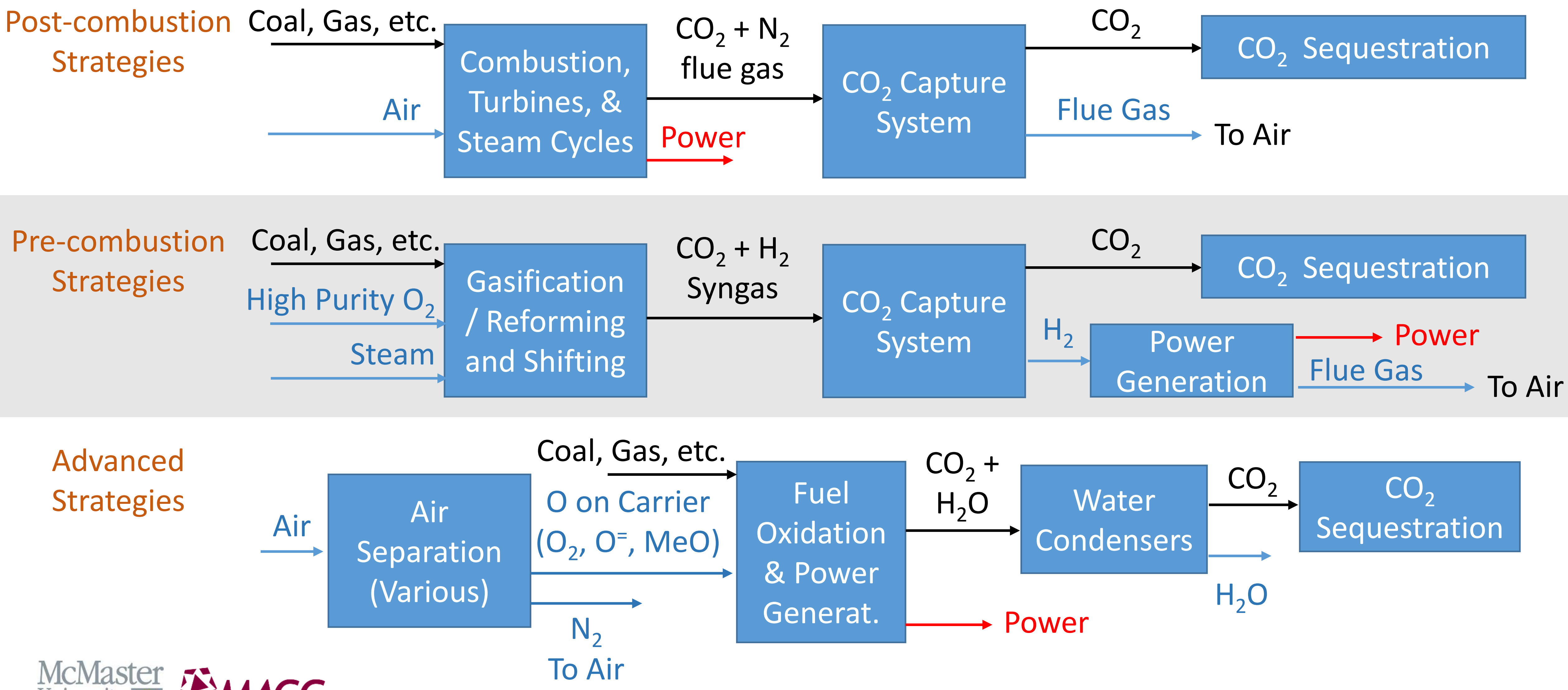
- Greenhouse Gases
- Particulates
- Deforestation
- Land Use / Transformation
- Resource Depletion
- Water Consumption
- Toxicity
- Wildlife Impact
- Noise

Societal

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

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

Motivation: Power Plant w/ CCS Comparisons



Motivation: Power Plant w/ CCS Comparisons

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

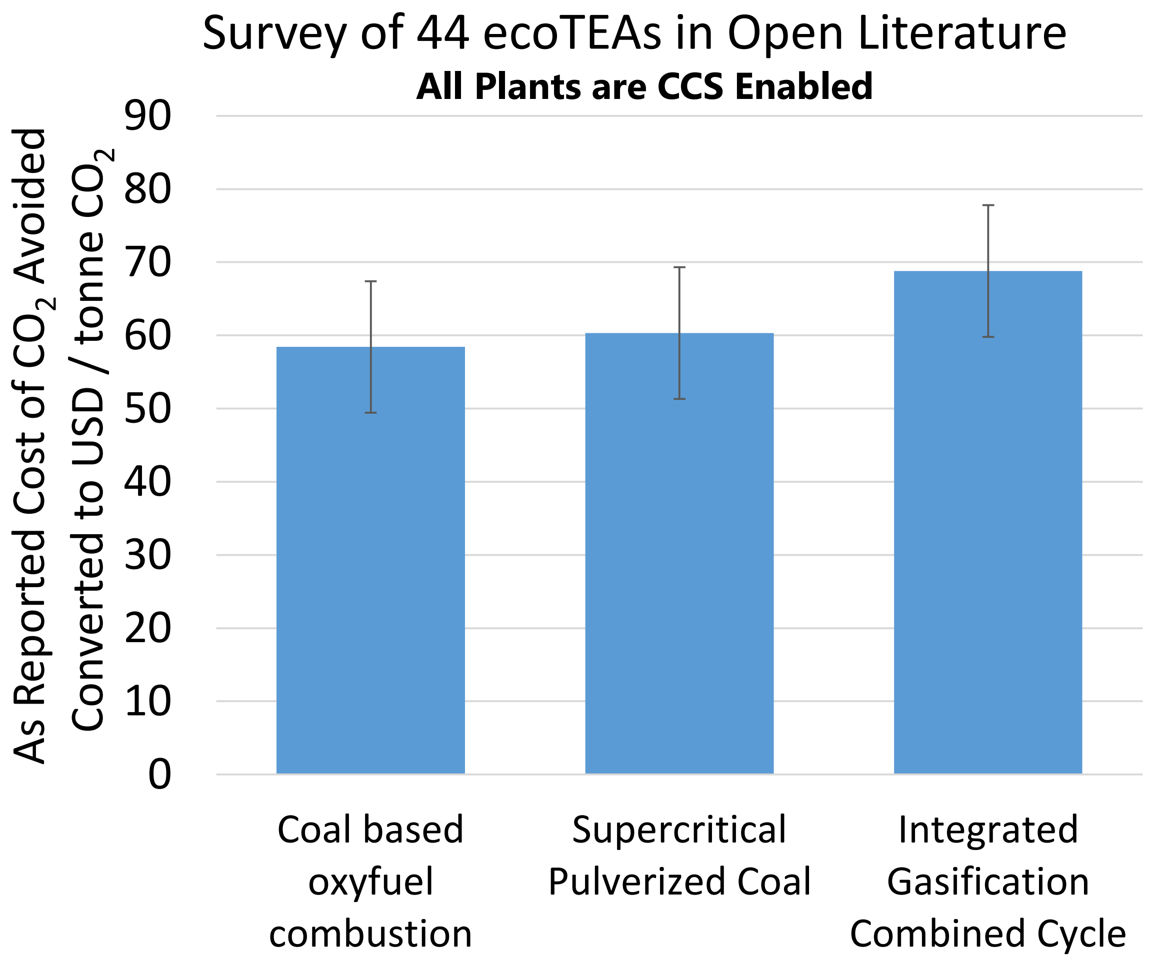
Key Problems

- No systematic comparison between processes
  - Lack of consistency between studies, especially between different author groups
- Everyone claims their own process is the best when compared against some other
  - Example: Don't compare against some common status quo, find another innovative idea that is worse and compare against that
- Wide variation in assumptions, strategies and ideas.
  - Different locations
  - Different definitions of key performance indicators
  - Different project years
  - Different analysis boundaries
- Cannot examine the literature to make fair comparisons between them.

Example of Literature Noise

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

- Disparity in GWP and LCOE computations
- Huge disparity in definition of the base case
- Yet this is a primary key performance indicator for identifying the best technologies to fight climate change

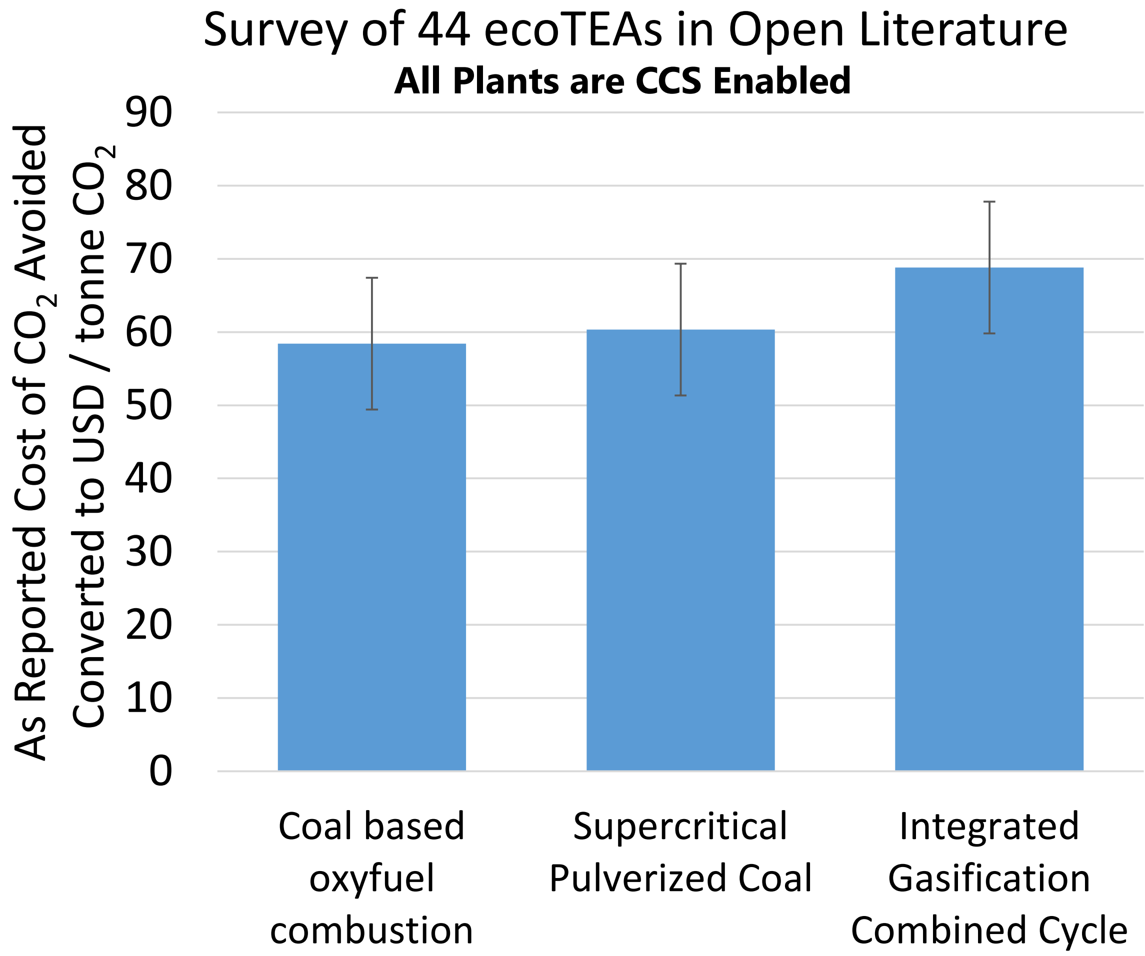


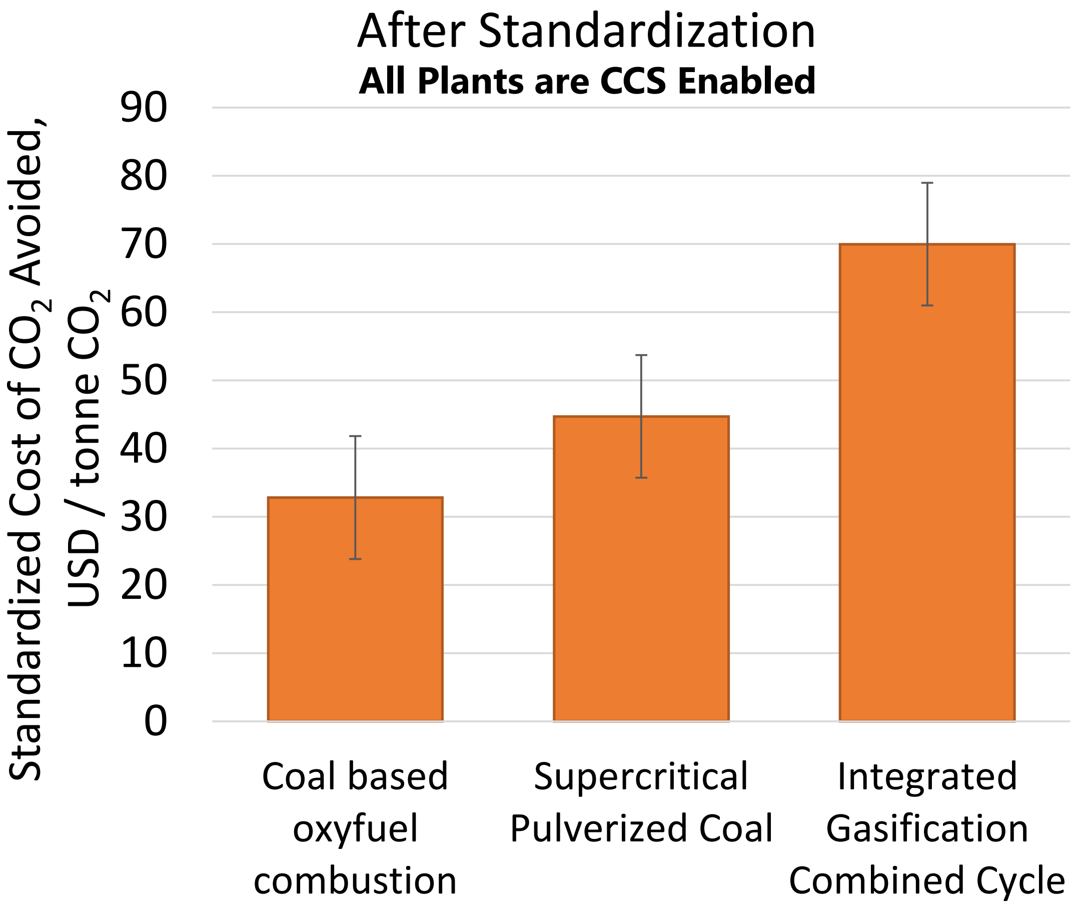
Notes: Error bars are for 90% Confidence Interval
Error bars assumes all power plants are equal within a category, which is not quite true, and so are for guidelines only.

Solution: Standardization

- 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

Example: After Standardization

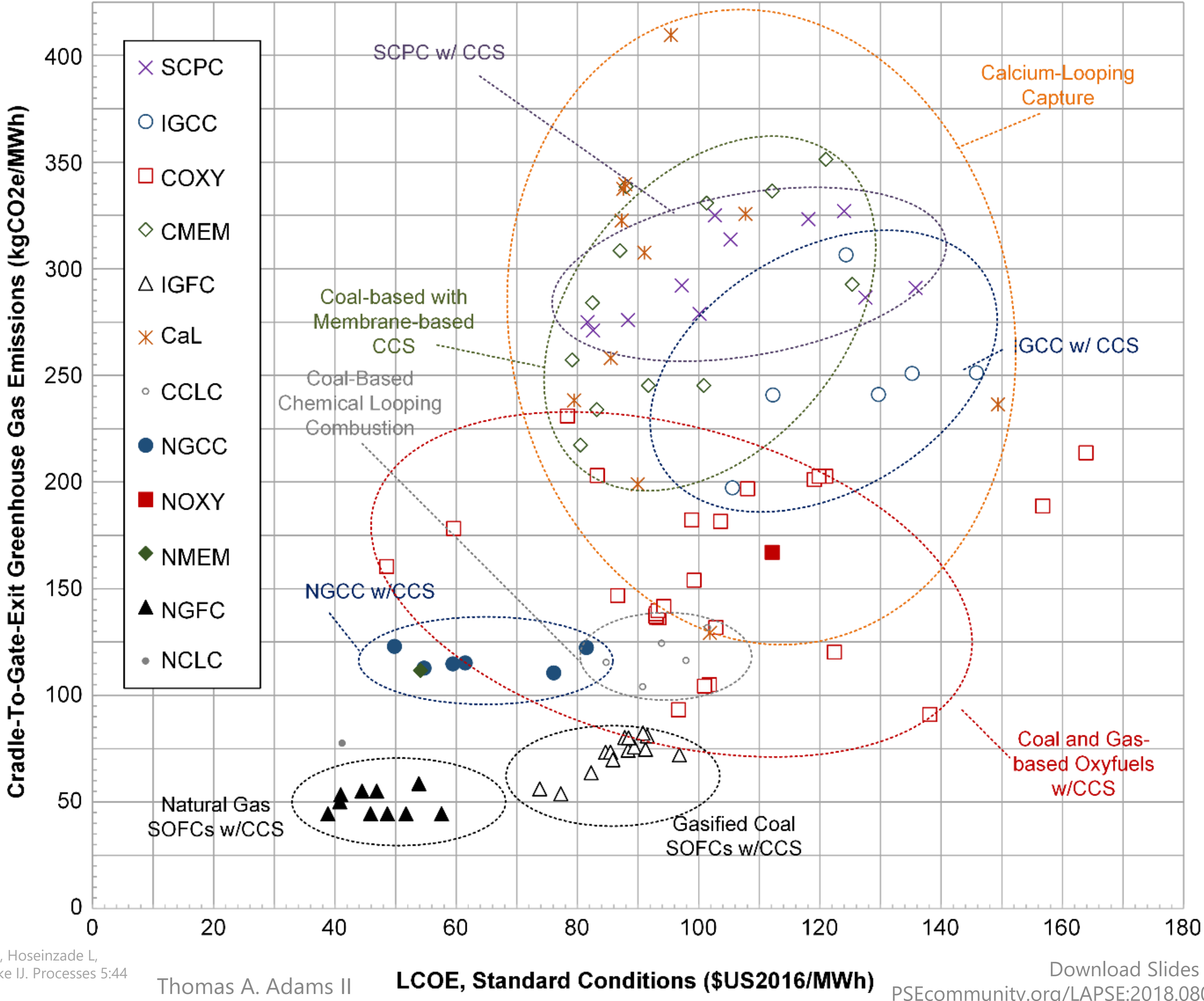




Notes: Error bars are for 90% Confidence Interval
Error bars assumes all power plants are equal within a category, which is not quite true, and so are for guidelines only.

Overall

- Clear trends emerge once standardized
- Able to group technologies into clear areas
- Macro-level comparisons are now possible.
- Value of the design concept now more evident



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

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Expanding and Standardizing

Big Picture Lessons from Study

- Rather hard to do cross-comparative research of eco-techno-economic analyses (eTEAs)

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

- But the rewards of doing meta-studies like this are significant

  Very useful society, business, and policy conclusions

- A standardization of eTEA methodology for the field would greatly amply the impact of each of our own studies

  Individual studies would have greater influence

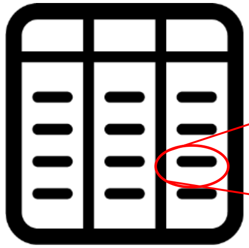
Proposal: Develop recognized standards for performing TEAs and eTEAs

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.

Standards Council of Canada
Conseil canadien des normes

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

$NPV_{alternate}$ = \$0.7 bln

$CCA_{alternate}$ = \$20.4/tonne

$GHG_{alternate}$ = 1.6 tCO_2e

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

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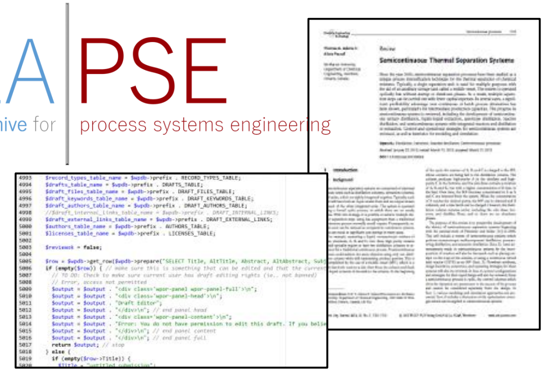

Paper Published. Models / spreadsheets / code released to public database

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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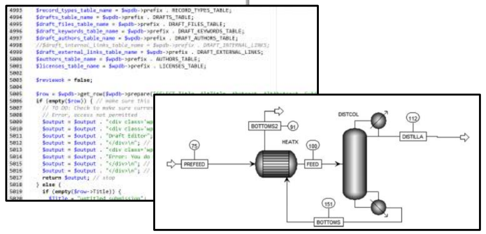
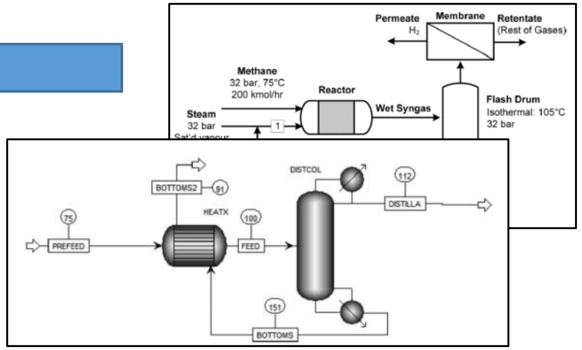


Reader downloads files and data to verify results

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!

Key Standards Characteristics (Goals)

Goals: Want standards that…

- result in unambiguous calculations that are directly comparable across research studies
- are useful
- are easy to use
- are transparent
  - transparency in reporting
  - transparency in calculations
  - ease of adoption
  - reproducible
- are international or regional
  - balance between breadth and detail
- are convertible
  - Example: metrics reported for a north American application easily converted to a European one.
- are accessible
  - digital reporting
  - standard meta data / tagging
  - databasing
  - open / cheap access of results

Standards Scope

Scope: eco-Technoeconomic analyses of energy systems.

- Applications:
  - Electricity
  - Transportation
  - Energy Conversion
  - Energy Product Production
  - Energy Storage
- Scales
  - Large
  - Neighbourhood
  - Personal

- Focus On:
  - Major system components
  - Important supply chain elements
  - Big-picture concepts
  - "Major on the majors"
- Avoid
  - Prescribing minutae
  - Too tight definitions and requirements

Key Definitions

Key Performance Indicators (KPIs)

- Common metrics of quality
- Potential Examples:

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

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

$GHG_{PSE\text{-}3}$ = 4.5 $MtCO_2e$/yr

$\eta_{therm,PSE\text{-}3}$ = 45.3% HHV

$PBP_{PSE\text{-}3}$ = 6.7 years

Intermediate Calculation Elements (ICEs)

- Used to compute KPIs
- Convertible from one standard basis to another. Example:

$TCI_{PSE\text{-}3}$ = \$1.11 billion USD

$TOC_{PSE\text{-}3}$ = \$123 million/yr USD

→ *(and others)* → $NPV_{PSE\text{-}3}$ = \$1.2 bln

↓ *Convert to PSE-3E Standard (Fuels, Large Scale, Europe)*

$TCI_{PSE\text{-}3E}$ = € 0.84 billion

$TOC_{PSE\text{-}3E}$ = € 95 million/yr

→ *(and others)* → $NPV_{PSE\text{-}3E}$ = € 0.94 bln

Example Standards: Size

- Size incredibly important! Example:
  - Same plants, 50% difference in size:

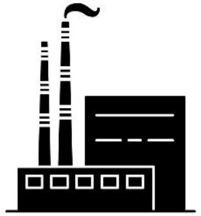
Pulverized Coal
w/CCS
550 MW
10.6 ¢/kWh
(standardized literature averages)

Pulverized Coal
w/CCS
225 MW
11.3 ¢/kWh
(standardized literature averages)

6.6% LCOE Difference

- Different plants, same size, standardized conditions

Pulverized Coal
w/CCS
550 MW
10.6 ¢/kWh
(standardized literature averages)



Coal Oxyfuel Combustion
w/CCS
550 MW
9.9 ¢/kWh
(standardized literature averages)

7.1% LCOE Difference

- The effect of size is equal to the effect of the process technology itself!
  - Need to control this variable in order to make technology value judgments.

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

And Yet We Do It All The Time

Common example

- Plant 1: 750 MW power plant without CCS

- Plant 2: 500 MW power plant with CCS

- Same Fuel Input
- CCS parasitic effect
  - But what about the remaining 250MW of power out! I want it!

LCA Concept of Functional Unit:

- Need to be outputs based
  - Comparisons should be based on like products and scales
  - BUT! Per-unit costs (like LCOE) are sensitive to size
    - Capital costs are non-linear (economies-of-scale)
    - i.e. power law scaling
  - We'll need to choose good size standards for comparison.
  - Environmental impacts are linear, so per-unit impacts are fine

Example Standards: Size

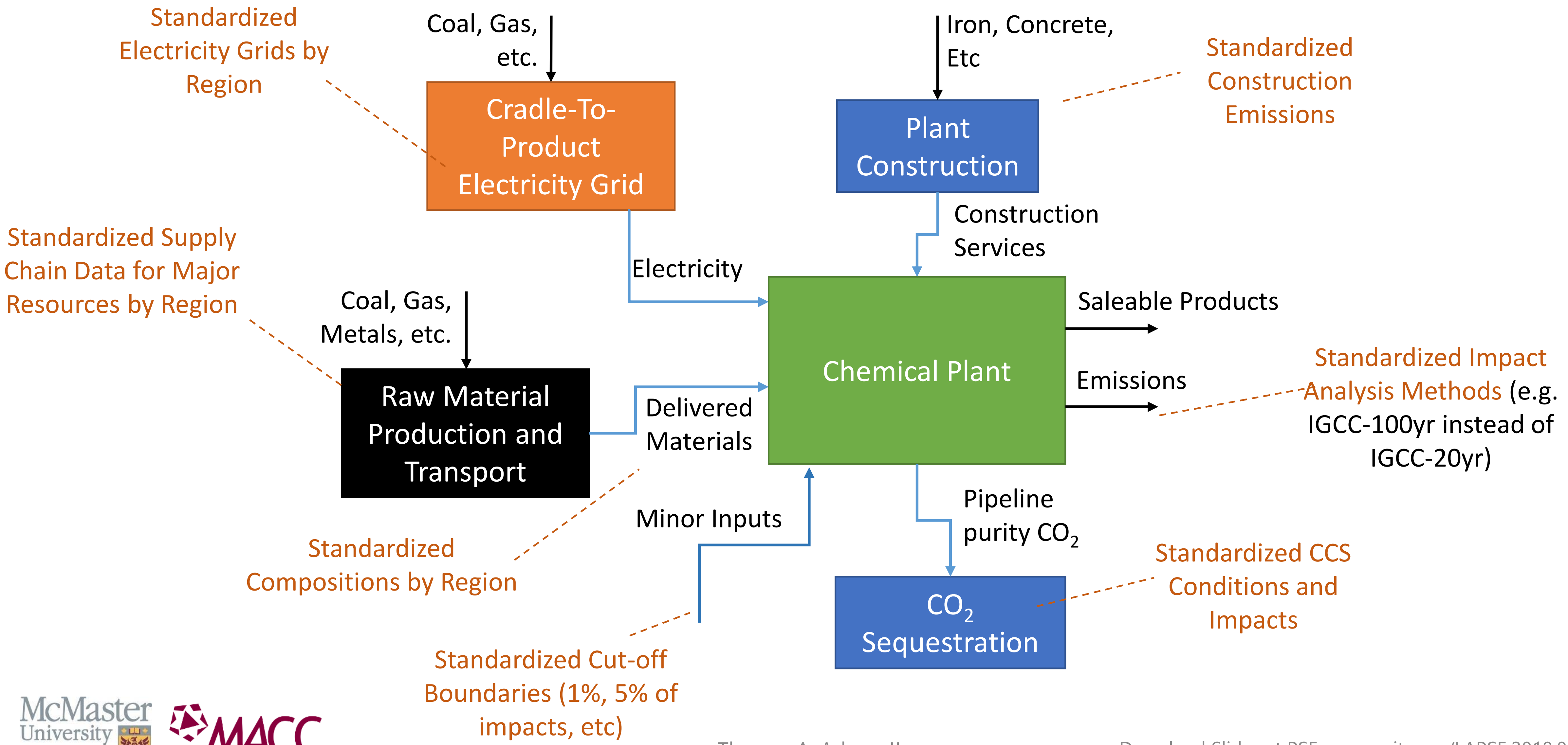
- User would choose which size standard to pick
  - Others could compare directly
  - Others could use Intermediate Calculation Elements to convert to their size of interest.

Size Standards by Category

PSE-1:	Electricity, Municipal	550 MW net output
PSE-2:	Electricity, Community	500 kW net output
PSE-3:	Electricity, Building	10 kW net output
PSE-4:	Fuels, Large plant	1 GW_{HHV} output
PSE-5:	Fuels, Small plant	10 MW_{HHV} output
PSE-6:	Transport, Personal	200,000 km
PSE-7:	Transport, Mass Transit	100,000 tonne-km

Etc. (*hypothetical numbers for sake of discussion*)

Example Standards: LCA Boundaries & Data



Example Standards: Regional Breakdown

*LCA Standards by Region for PSE-1 (*Electricity, Municipal). Electricity Grid Cradle-to-Product Emissions

Basis: 1 MWh Electricity, AC, grid quality, delivered		CO_2 (*kg/MWh*)	NO_X (*kg/MWh*)	CH_4 (*kg/MWh*)	GWP (*kgCO2e/MWh*)
PSE-1N:	North America	655	1.63	2.62	728
PSE-1E:	Central Europe	500	1.11	1.31	537
PSE-1S:	South America	157	0.37	0.93	183
Etc.	…	…	…	…	…

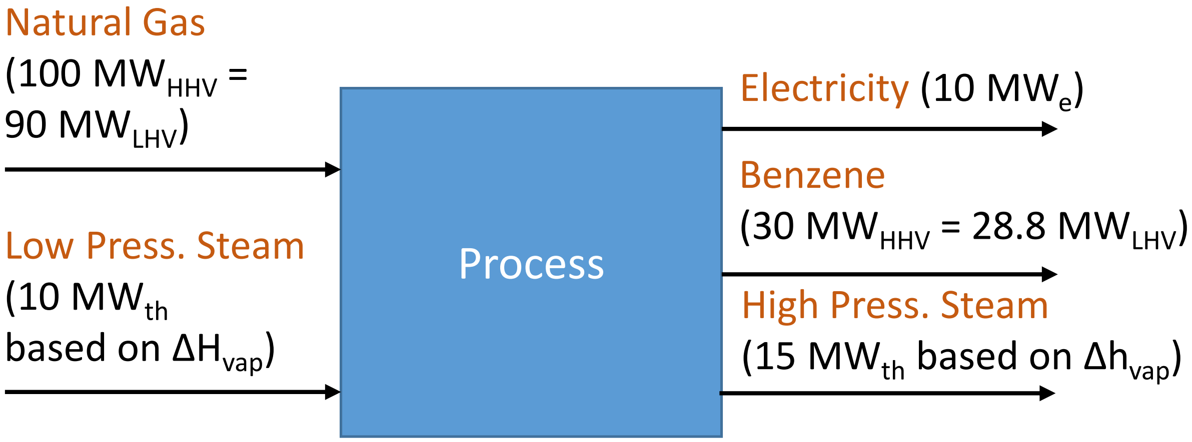
Similar tables would exist for many aspects of the supply chain

Numbers hypothetical for sake of discussion / do not use.
Approximated based on citations below.

Sources: Jiminez-Gonzalez C, Constable DJC. Green Chemistry and Engineering: A Practical Design Approach. Wiley. pg 527 (2011)
IPCC 5th Assessment
Barros MV, Piekarski CM, de Francisco AC. Energies. 11:1412 (2018)

Example Standards: Metrics

- Example: Efficiency. What is the efficiency of this system? Which do you report?



Is the steam energy just Δh_{vap} ?
Does it include specific heat effects?
Does it include pressure effects?

Do you use LHV or HHV?

How do you add electric, thermal, and chemical energies?

$$\eta = \frac{benzene\ (primary\ product)}{gas\ (raw\ material)}$$

$$\eta = \frac{all\ saleable\ products}{gas\ (raw\ material)}$$

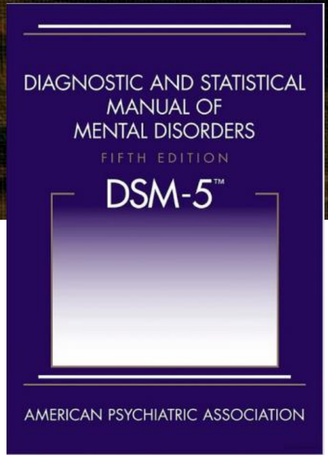
$$\eta = \frac{all\ saleable\ products}{all\ inputs}$$

$\eta = 30\%_{HHV}$ $\eta = 32\%_{LHV}$

Without specific heat/pressure counted: $\eta = 55\%_{HHV}$ $\eta = 60\%_{LHV}$ — $\eta = 50\%_{HHV}$ $\eta = 54\%_{LHV}$

With specific heat/pressure counted: $\eta = 56\%_{HHV}$ $\eta = 61\%_{LHV}$ — $\eta = 51\%_{HHV}$ $\eta = 55\%_{LHV}$

Example Standards: Transparency



- New DSM-5 medical anxiety conditions*:

Aspen·alium·errata·phobia	Fear of others finding mistakes in your Aspen Plus models
Aspen·alium·quæstrum·iniquumo·phobia	Fear of others taking your Aspen Plus models and publishing papers with them really fast even though it took you, like, a year to make!

- Recent review of over 300 papers which use energy systems modelling found just 3 released their models to the public.

* Not really of course

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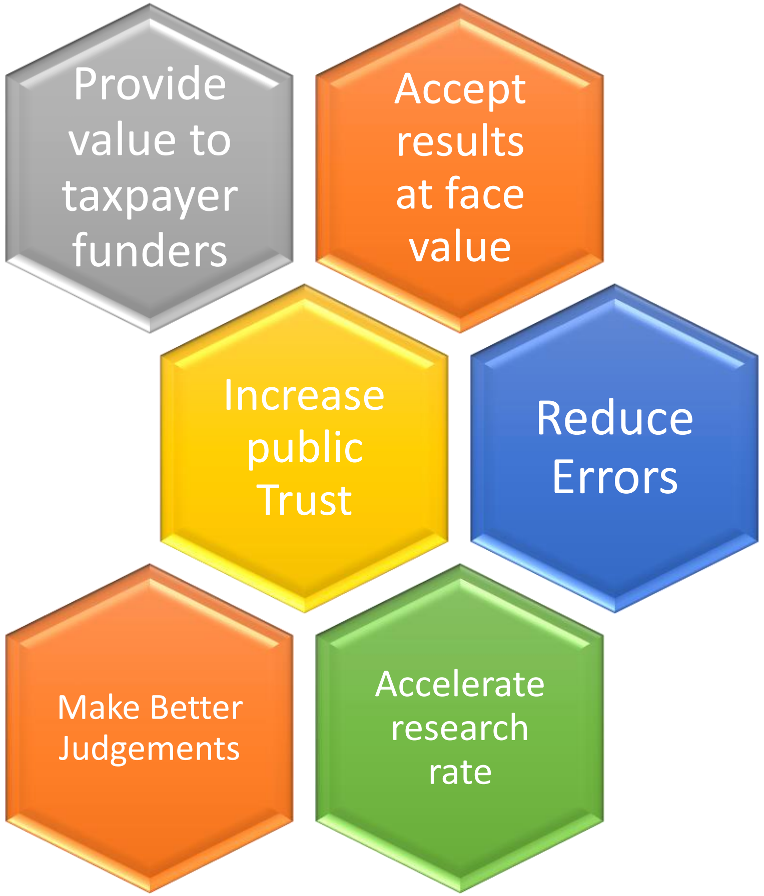
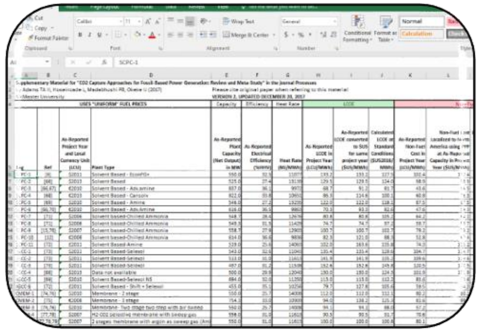
Source: Subramanian ASR, Gundersen T, Adams TA II. Processes 6:238 (2018)

Example Standards: Transparency

Goals



Techniques

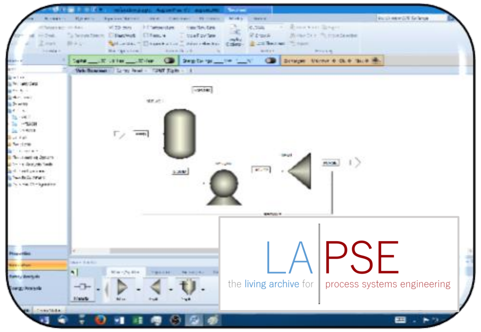


Spreadsheets

- With formulas!
- As journal supplementary material

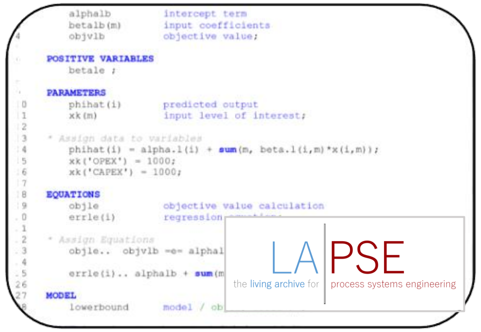
Source Code (.py, .cpp, .m)

- Compliable for non-experts
- Binaries too
- GitHub, CodeBase, LAPSE



Simulations and Flowsheets

- Converged
- CAPE-OPEN compliant
- LAPSE



Optimization

- GAMS code
- LAPSE
- Journal supplementary material

Similar Standards Movements

- NETL/US DOE: Quality Guidelines for Energy Systems Studies
  - Internal / recommended
    - Modeling params (e.g. Aspen models)
    - Economic (e.g. debt/equity ratios)
    - Fuel standards (e.g. gas quality, price)
  - Used in making the "baseline" studies
  - Can help to address some standardization elements
  - Some likely to be adopted in proposed standard
  - USA Focused. A great start!

- ISO 14040 series
  - Life Cycle Analyses
  - Boundaries and Guidelines
  - Not specific enough for standardization
  - Incorporate as best practices
- ISO 50006/50015/17741
  - Energy management systems
  - Defines metrics like efficiency
  - Useful terminology
  - Analysis boundary definitions
  - Some portions incorporated
  - But eTEAs out of scope

Similar Standards Movements (continued)

- White paper: Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization (2018)
  - Technische Universität Berlin
  - RWTH Aachen University
  - Univ Sheffield
  - Institute for Advanced Sustainability Studies eV Potsdam
  - University of Michigan

- Proposes TEA standards in a parallel way to ISO 14040+ life cycle analysis standards
  - A similar best-practices theme
  - Means not specific enough for the cross-research results application
  - Scope too specific/narrow
  - Well thought out and described
- An excellent start
  - Much that could be included in or greatly inform new ISO standard

Standardization Committees and Process

- Stage 1 (Now)
  - Letters of support from universities, companies and agencies
    - no commitments
    - no money
  - You can help by sending me a letter of support on your letterhead
    - Template available at link below
  - Interested? Join the mailing list at
    - http://PSEcommunity.org/standards

- Stage 2
  - Standards Council of Canada will compile and create proposal to ISO

Standards Council of Canada
Conseil canadien des normes

  - Once approved, technical committee formed
  - Mirror committees will be formed by participating countries. Join!

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!
  - http://PSEcommunity.org/standards