# Eco-Technoeconomic Analyses for Industrial Process Systems

# New Work Item Proposal for a Technical Specification

Chemical Institute of Canada | ***For Our Future***
Institut de chimie du Canada | ***Pour notre avenir***

# What is Standardized Eco-Technoeconomic Analyses (eTEAs)?

**eTEA:**
A Methodology for determining Important Metrics about Industrial Processes

**Eco**
- Environmental Impacts
- LCA / LCIA / etc.

**Techno**
- Materials and Energy Flows
- Efficiencies

**Economic**
- Costs / Profitability
- Uncertainty / Risk

# Key Users of eTEAs:

| Chemical & Energy Industry | Capital Finance | Funding Agencies | Academic Research |
|---|---|---|---|
| • Technology selection<br>• Process Design Decisions<br>• Go/No-go decisions<br>• Business Plan | • Risk Assessment<br>• Interest Rate Determination<br>• Project Valuation<br>• New: Green Finance | • Assessment of Merit<br>• Environmental Impacts<br>• Cross-cutting comparisons | • Conceptual Design<br>• Early Research Valuation<br>• Technology Potential<br>• Policy Advice |

# Why do we need an eTEA Technical Specification?

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

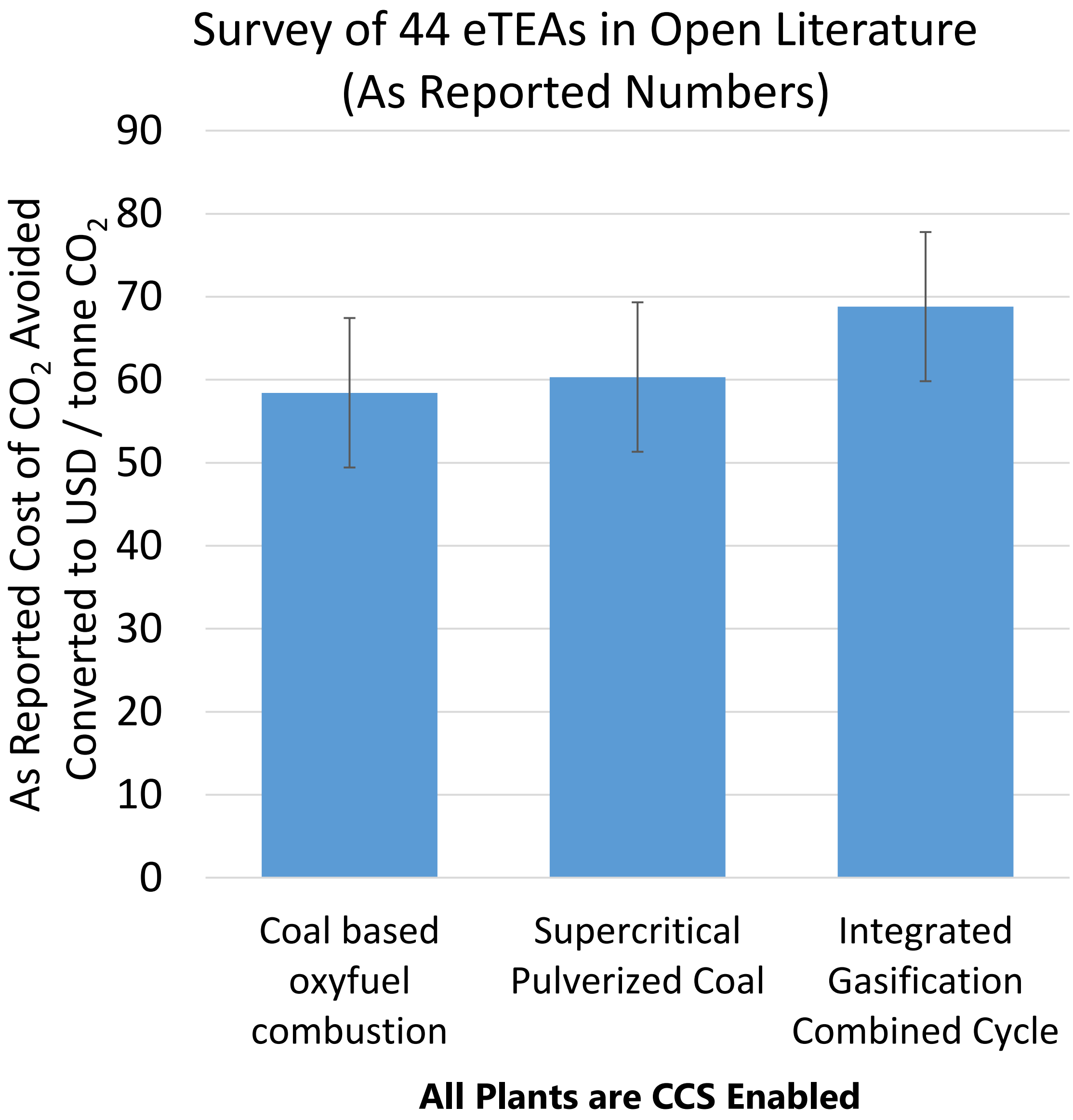
- Easy to set up a “straw man” argument

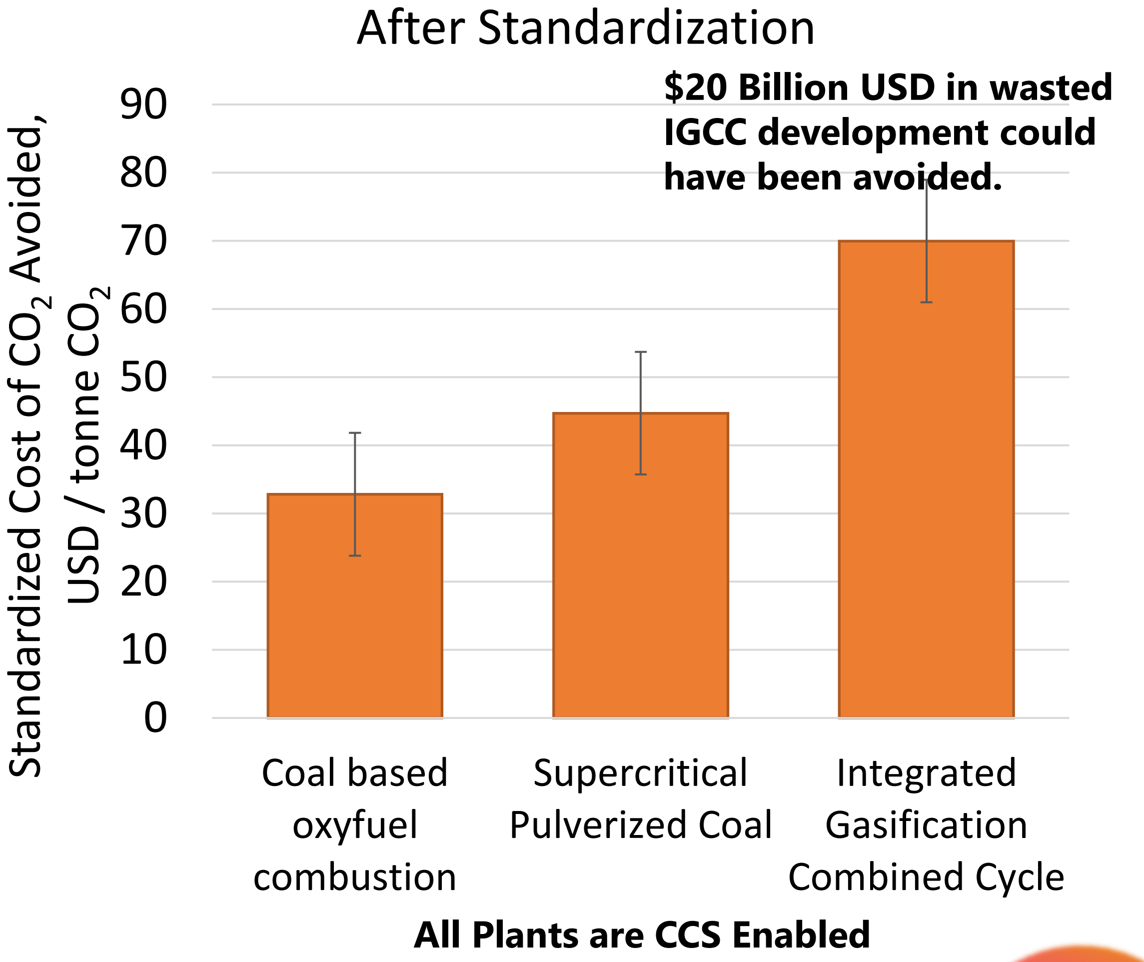
Wide variation in assumptions, strategies and ideas.

- Different locations
- Different definitions of key performance indicators
- Different project years
- Different analysis boundaries
- Different supply chains
- Different sizes

**Cannot examine the literature to make fair comparisons between studies.**

# Simple Example: Standardization Impacts



# Scope: Industrial Chemical and Energy Processes

The proposed technical specification (TS) would provide definitions, processes and guidance for the application of different methodologies for performing an eco-technoeconomic analysis (eTEA). The TS will primarily define:

### Applications

- Electricity
- Transportation Fuels
- Energy Conversion
- Energy Production
- Energy Storage
- Chemicals

### Scales

- Large
- Neighbourhood
- Personal

### Key Performance Metrics (KPIs)

- Net Present Value
- Levelized Cost of Electricity
- Minimum Selling Price
- Life Cycle Environ-mental Impacts (GHGs, Smog, Acid Rain, etc.)
- Cost of $CO_2$ Avoided
- Efficiency of various kinds

### Standard Parameters

- Process size or scale
- Point of Comparison
- LCA boundaries
- GHG equivalency tables
- Financial parameters
- Fuel Price / Supply Chain
- Time and Place of Comparison

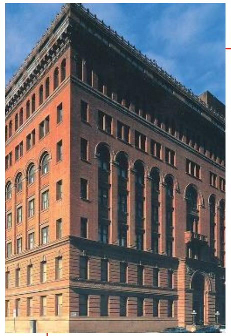
# Key Benefits

## Chemical and Energy Industry

- Better technology decision-making
- Reduced costs of borrowing
- Improved analyst and engineer training

## Capital Finance

- Reduced risks
- Better transparency
- Enhanced green finance regulations



## Funding agencies

- Better use of public funds
- Higher success rates
- Reduced biases and hype

## Researchers

- Higher impacts
- Cross-cutting analysis
- Rapid research

## Society

- Lower cost goods
- Lower environmental footprints
- Better public policy

# Similar Movements outside ISO

- 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!

- White paper: Techno-Economic Assessment & Life Cycle Assessment Guidelines for $CO_2$ Utilization (2018)
  - Technische Universität Berlin
  - RWTH Aachen University (André Bardow)
  - Univ Sheffield
  - Institute for Advanced Sustainability Studies eV Potsdam
  - University of Michigan
  - Proposes TEA standards in a parallel way to ISO 14040+

# Why TC 207/SC5 ?

- ISO 14040+ provides generalized framework
- This is the inevitable extension and application of that
  - Proposed methods still fall under ISO 14040+ thinking and are used in most cases
  - We need to be specific on certain, selective things only
- This relies on the concept of functional unit
  - Not commonly done for TEAs (which is why the problem exists)
- Need the expertise of this committee on LCA principles first and foremost

# Global Supporters

- **Belgium**
  - Vrije Universiteit Brussel
- **Canada**
  - Canadian Society for Chem. Eng. *(Champion)*
  - McMaster University *(Champion)*
  - Queens University *(Champion)*
  - Ryerson University
  - University of Waterloo
  - University of Calgary
  - University of Toronto
  - University of Ontario Institute of Technology
- **Germany**
  - Technical University of Berlin
  - RWTH Aachen
  - Ostbayerische Technische Hochschule Regenburg
- **India**
  - IIT Roorkee *(Champion)*
- **Japan**
  - Tohoku University
- **Norway**
  - Norges teknisk-naturvitenskaplige universitet
- **Spain**
  - UPC Universitat Politècnica de Catalunya
  - IMDEA
- **South Korea**
  - Pukyong National University *(Champion)*
- **USA**
  - Eastman Chemical Company *(Champion)*
  - Massachusetts Institute of Technology *(Champion)*
  - University of Wisconsin *(Champion)*
  - West Virginia University *(Champion)*
  - US Environmental Protection Agency
  - US Department of Energy
  - Texas A&M University
  - University of Texas
  - North Carolina State
  - Exxon Mobil
- **United Kingdom**
  - Aveva

# What’s Next?

- ISO has opportunity to fill key gaps in eTEAs
- We need ISO member support
- Subject experts needed to help develop Technical Specification
- Technical Specification will be regionalized—different parameters for different regions of applications
  - Example: supply chain of natural gas very different in North America vs East Asia

Questions?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# Additional Slides / Extra Information

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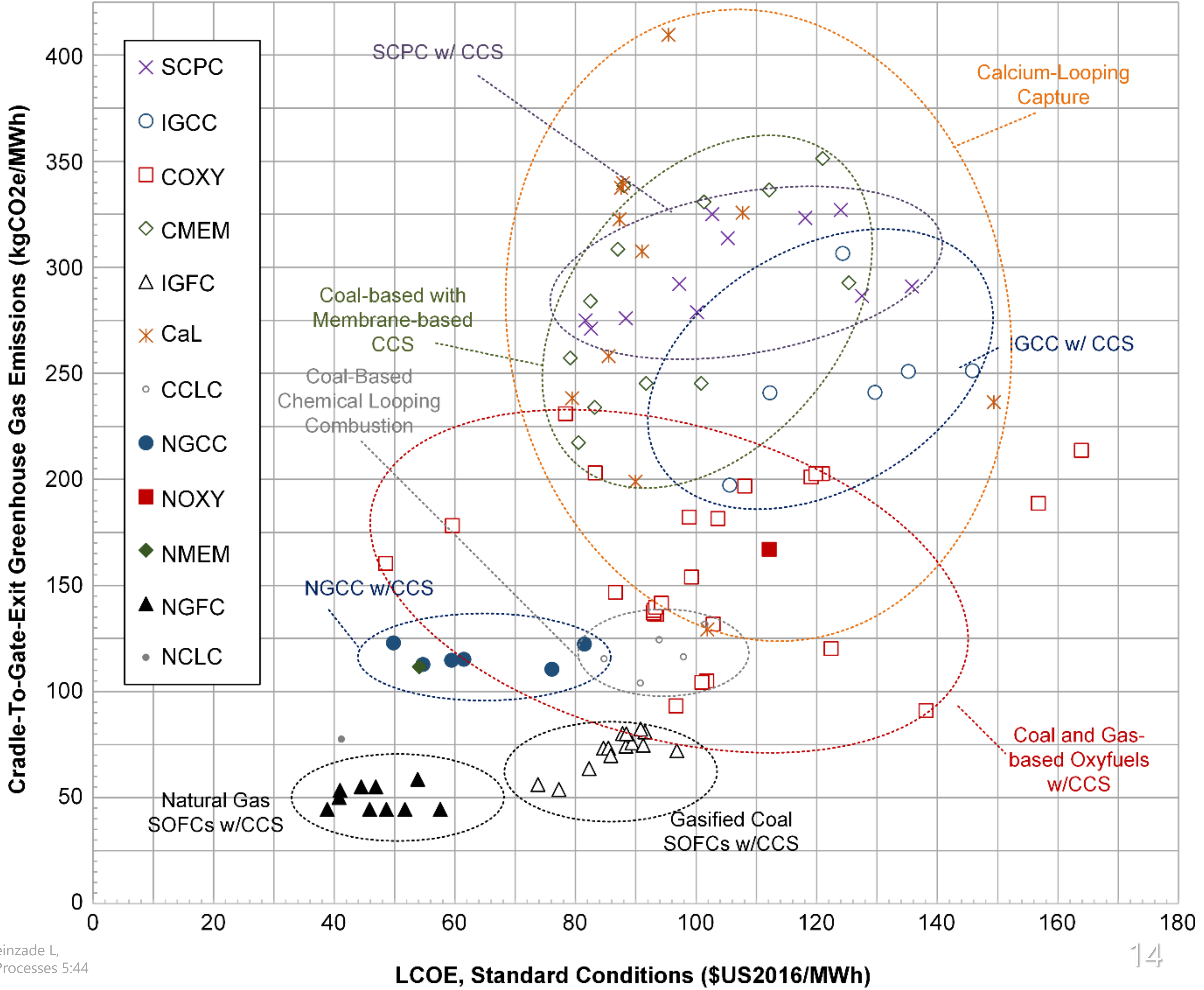
# Example: North American Power Plants

- 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

- 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




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

# 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*

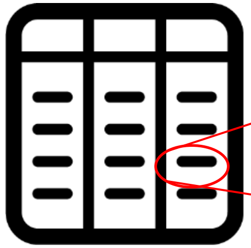
*Individual studies would have greater influence*

# Example of Parameters to be Standardized

| 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: Analysts

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

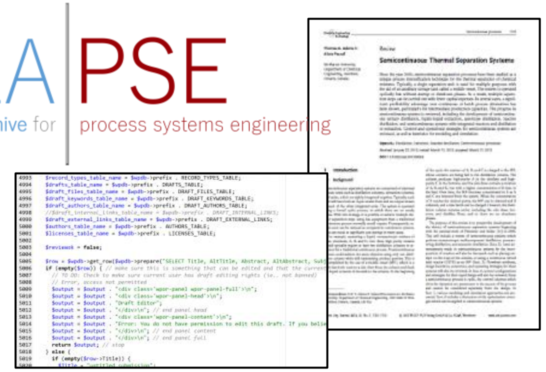
$NPV_{alternate}$ = \$0.7 bln

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

$GHG_{alternate}$ = 1.6 $tCO_2e$

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

LA | PSE
the living archive for process systems engineering



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

# Example Use of Standards: Readers

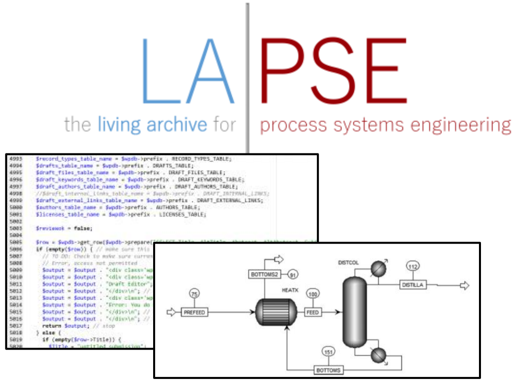
Reader views paper using PSE standard

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

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

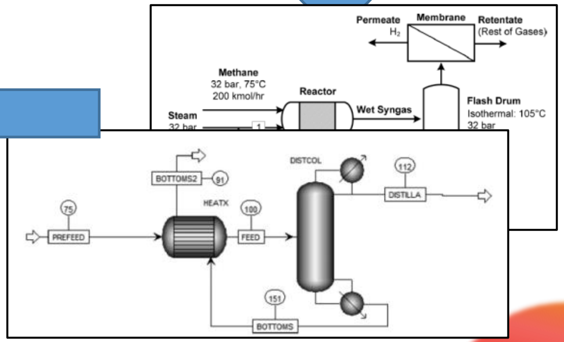
$GHG_{PSE\text{-}3}$ = 4.5 $tCO_2e$

Reader sees standard metrics, immediately understood




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 analysis

Better & faster results. More meaningful insights!

# Industrial Benefits and Involvement

- Anticipated Industrial Role:
  - Not expected to release in-house studies or codes to the public, IP, etc.
  - Seen as consumer of academic / government data, not producer
  - Key stakeholder involvement in standards process
    - Need to know what is most valuable aspects
    - What baselines of comparison should we be using
    - What financial parameters, etc.

- Potential Industrial Benefits
  - Better in-house greenlight decision making
  - Faster data gathering and interpretation
  - Easier training of employees
    - (Anticipated that standard will become ABET/CEAB accreditation requirement for chem eng design courses)
  - Improved client confidence
    - Capital lenders may consider reduced risks of decisions when made based on standardized methodologies
    - Increased client trust (internal/external) in project estimates and projections

# 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

# 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:

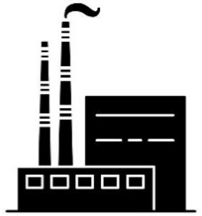
Pulverized Coal
w/CCS
550 MW
10.6 ¢/kWh
(standardized literature averages)

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

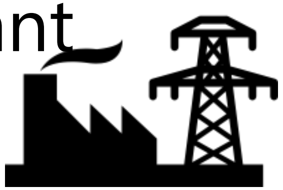
- The effect of size is equal to the effect of the process technology itself!
  - Need to control this variable in order to make technology value judgments.

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

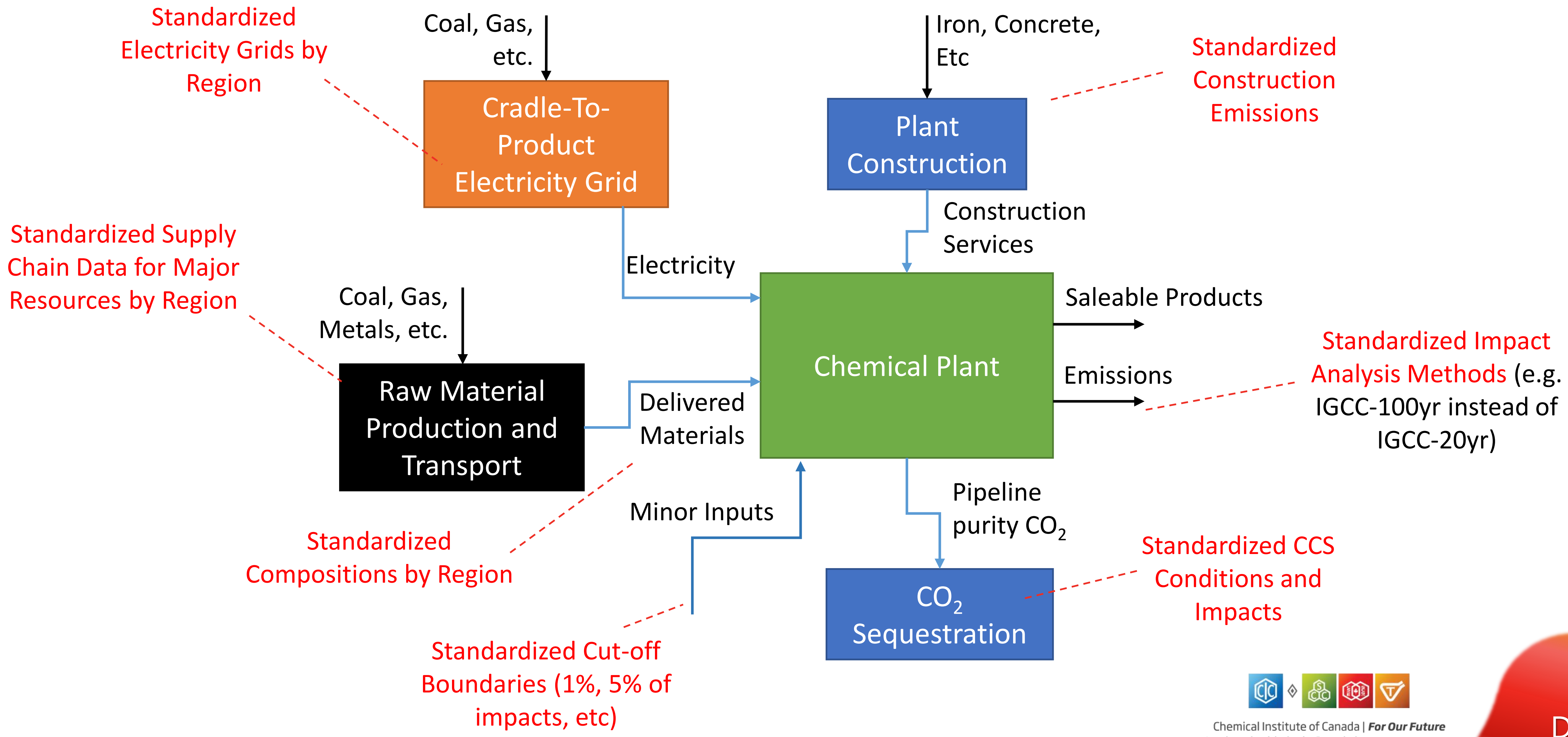
- User would choose which size standard to pick
  - Others could compare directly
  - Others could use Intermediate Calculation Elements to convert to their size of interest.

*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.* | … | … | … | … | … |

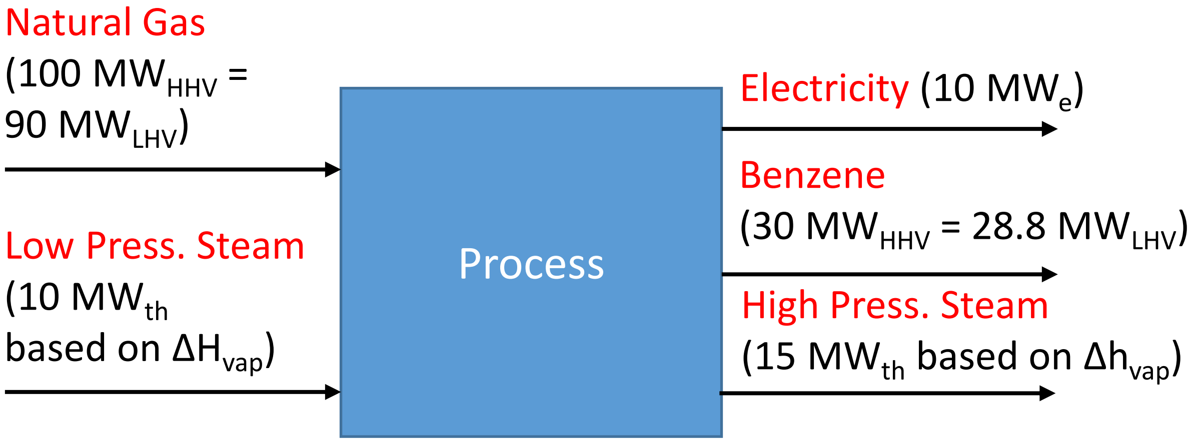
Similar tables would exist for many aspects of the supply chain

*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 $\Delta h_{vap}$ ?
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?

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

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

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

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

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

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

$\eta = 50\%_{HHV}$ $\eta = 54\%_{LHV}$

$\eta = 51\%_{HHV}$ $\eta = 55\%_{LHV}$

# 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 (André Bardow)
  - 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



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# For More Info: White Paper and Lecture

- A short 6-page proposal has been prepared
- Published in *Computer Aided Chemical Engineering* (paywalled)
- Ask me for a free copy
- Detailed technical presentation on the proposed standard (45 mins)

http://psecommunity.org/standards


Salvador Garcia Muñoz, Carl Laird, Matthew Realff (Eds.)
Proceedings of the 9th International Conference on Foundations of Computer-Aided Process Design
July 14th to 18th , 2019, Copper Mountain, Colorado, USA. 
http://dx.doi.org/10.1016/B978-0-12-818597-1.50057-6

## MAXIMIZING OUR IMPACT: A CALL FOR THE STANDARDIZATION OF TECHNO-ECONOMIC ANALYSES FOR SUSTAINABLE ENERGY SYSTEMS DESIGN RESEARCH

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*Abstract*

The literature is rich with interesting process design concepts, innovative ideas, and diverse approaches to designing energy systems within a sustainability mindset. However, there is no standard way of performing "eco-techno-economic" analyses in such a way that the results of different studies can be directly compared against each other in a meaningful way without significant effort. This makes it difficult to decide which process concepts are the best choices for further research, development, and investment. Therefore, I propose the development of a standardized methodology for eco-techno-economic analyses that would include a standard collection of metrics and associated computation methodologies; standard sizes, geographic locations, and applications of energy systems; standard "status-quo" baselines for comparison purposes; standard supply chains with which to conduct life cycle analyses; and open-access to computer models and data. These standards would be developed over time by an international committee of process systems engineering researchers and practitioners, interface with existing standards such as CAPE-OPEN and life cycle analysis standards, and ultimately lead to a new and continually maintained international standard. All future research studies which adhere to such standards would then be significantly more impactful since they could be directly and immediately validated, compared, adopted, reused, augmented, and understood in the larger research context.

*Keywords*

Sustainability, Energy Systems, Process Design, Techno-Economic Analyses, Standards, Methodologies.

### Introduction

The process systems engineering (PSE) community has been very active in the conceptual process design of sustainable energy systems. These systems include the production of transportation fuels, synthetic fuels, alternative fuels, alcohols, ethers, olefins, electricity, chemical energy storage carriers, and many other factors, with applications large and small. The sustainability aspect typically focuses on ways of decreasing greenhouse gas emissions but also can include other environmental factors such as water, food, smog, acid rain, and many others. For example, a recent review by Subramanian et al. (2018) studied over 300 recent publications just on the modeling and simulation aspect of energy systems (out of over 5000 publications identified since 2015), showing a considerable amount of activity.

However this is in stark contrast to the commercial activity related to the construction of novel sustainable energy systems. Despite all of the advanced conceptual designs put forward, very few new process design concepts have been successfully commercialized within the past decade. Some

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