Modernizing the Undergraduate Process Design Curriculum

Recommendations for CAChE and everyone else

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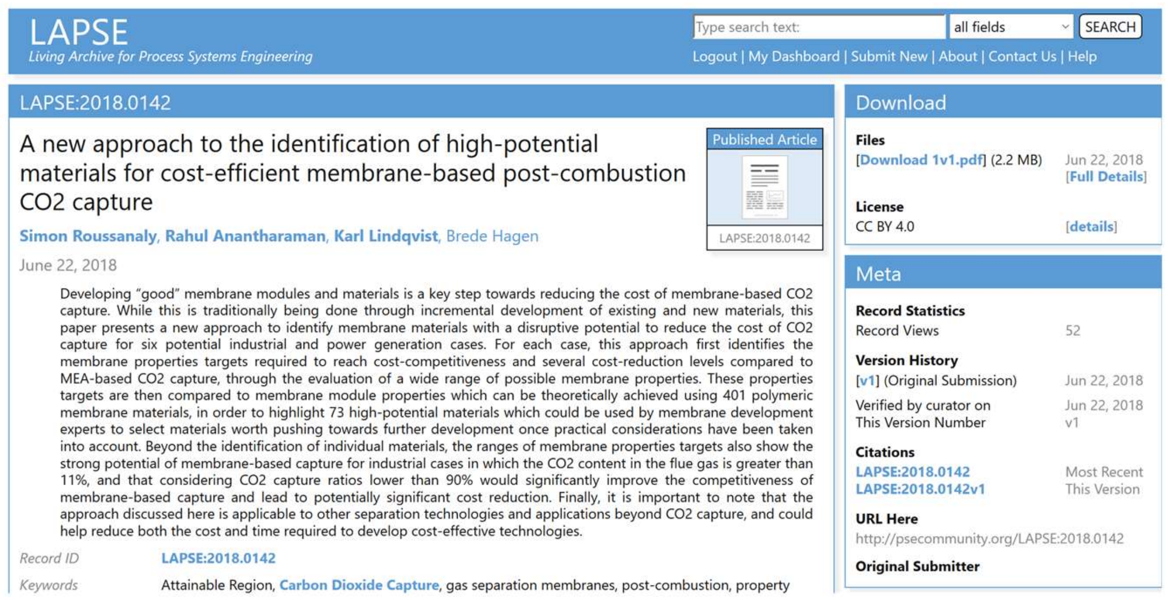

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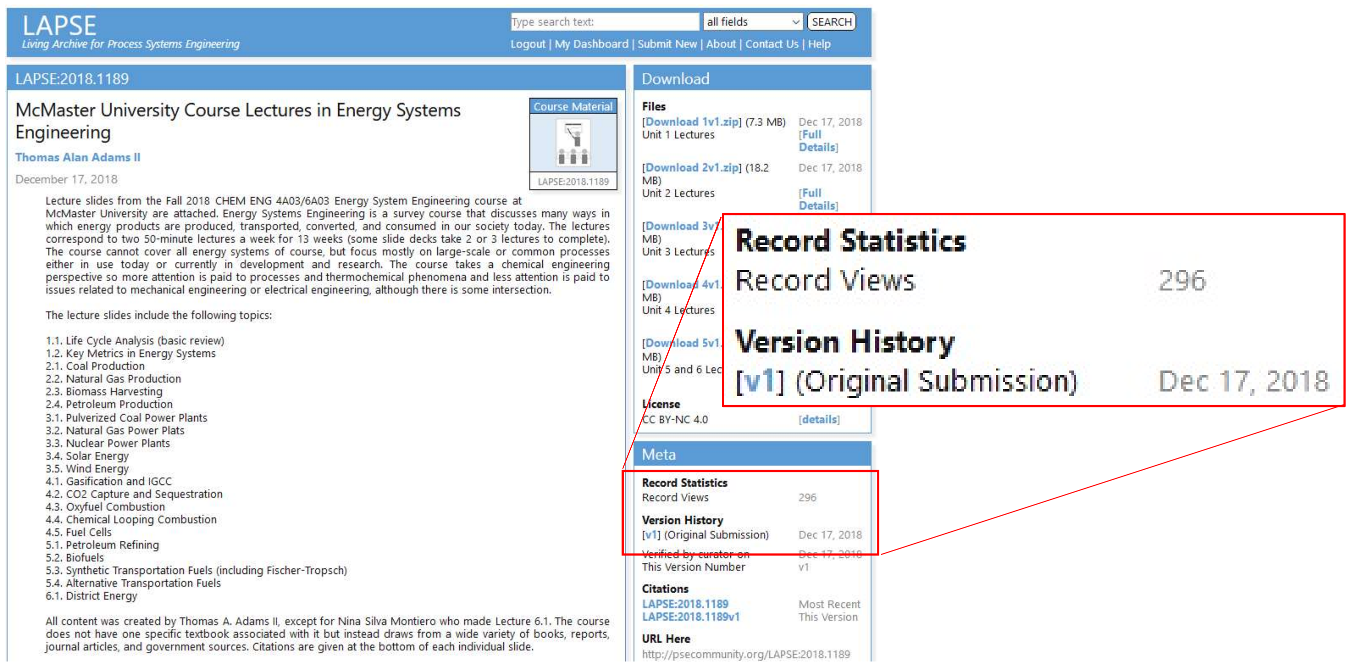

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Published Article

LAPSE:2019.0638

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Highly Selective Syngas/H2 Production via Partial Oxidation of CH4 Using (Ni, Co and Ni–Co)/ZrO2–Al2O3 Catalysts: Influence of Calcination Temperature

Anis Hamza Fakeeha, Yasir Arafat, Ahmed Aidid Ibrahim, Hamid Shaikh, Hanan Atia, Ahmed Elhag Abasaeed, Udo Armbruster, Ahmed Sadeq Al-Fatesh

July 17, 2019 (v1)

Subject: **Reaction Engineering**

Keywords: Al2O3, bimetallic catalyst, methane, partial oxidation, **Syngas**, ZrO2

In this study, Ni, Co and Ni–Co catalysts supported on binary oxide ZrO2–Al2O3 were synthesized by sol-gel method and characterized by means of various analytical techniques such as XRD, BET, TPR, TPD, TGA, SEM, and TEM. This catalytic system was then tested for syngas respective H2 production via partial oxidation of methane at 700 °C and 800 °C. The influence of calcination temperatures was studied and their impact on catalytic activity and stability was evaluated. It was observed that increasing the calcination temperature from 550 °C to 800 °C and addition of ZrO2 to Al2O3 enhances Ni metal-support interaction. This increases the catalytic activity and sintering resistance. Furthermore, ZrO2 provides higher oxygen storage capacity and stronger Lewis basicity which contributed to coke suppression, eventually leading to a more stable catalyst. It was also observed that, contrary to bimetallic catalysts, monometallic catalysts exhibit higher activity with higher calcination temperatur... [more]

Published Article

LAPSE:2019.0637

2. LAPSE:2019.0637

On the Use of Starch in Emulsion Polymerizations

Shidan Cummings, Yujie Zhang, Niels Smeets, Michael Cunningham, Marc A. Dubé

July 17, 2019 (v1)

Subject: **Interdisciplinary**

Keywords: emulsion, graft, polymerization, polysaccharide, Starch

Curated Subjects & Keywords

The substitution of petroleum-based synthetic polymers in latex formulations with sustainable and/or bio-based sources has increasingly been a focus of both academic and industrial research. Emulsion polymerization already provides a more sustainable way to produce polymers for coatings and adhesives, because it is a water-based process. It can be made even more attractive as a green alternative with the addition of starch, a renewable material that has proven to be extremely useful as a filler, stabilizer, property modifier and macromer. This work provides a critical review of attempts to modify and incorporate various types of starch in emulsion polymerizations. This review focusses on the method of initiation, grafting mechanisms, starch feeding strategies and the characterization methods. It provides a needed guide for those looking to modify starch in an emulsion polymerization to achieve a target grafting performance or to

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Published Version [10.1016/j.ijhydene.2017.08.031]

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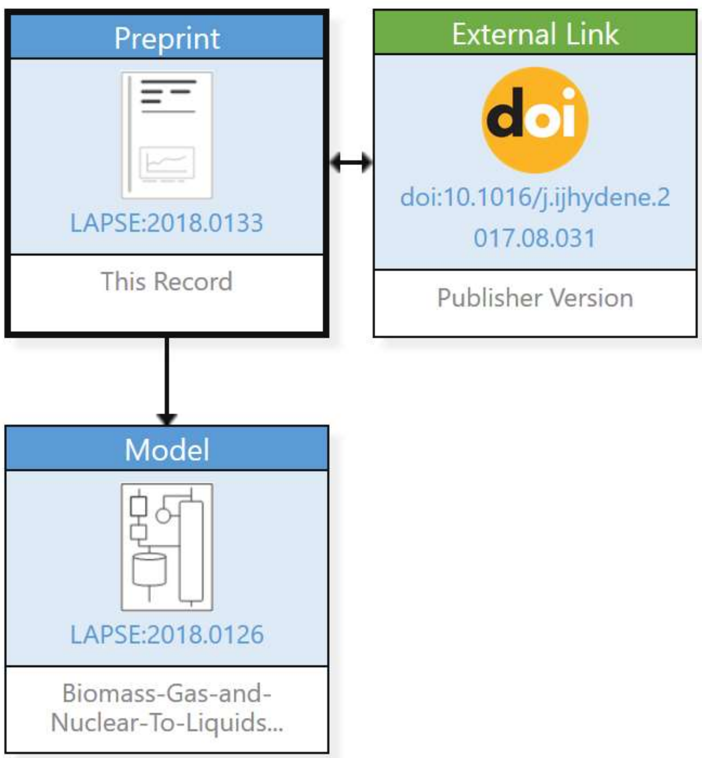

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- Connect to the work of others as well.
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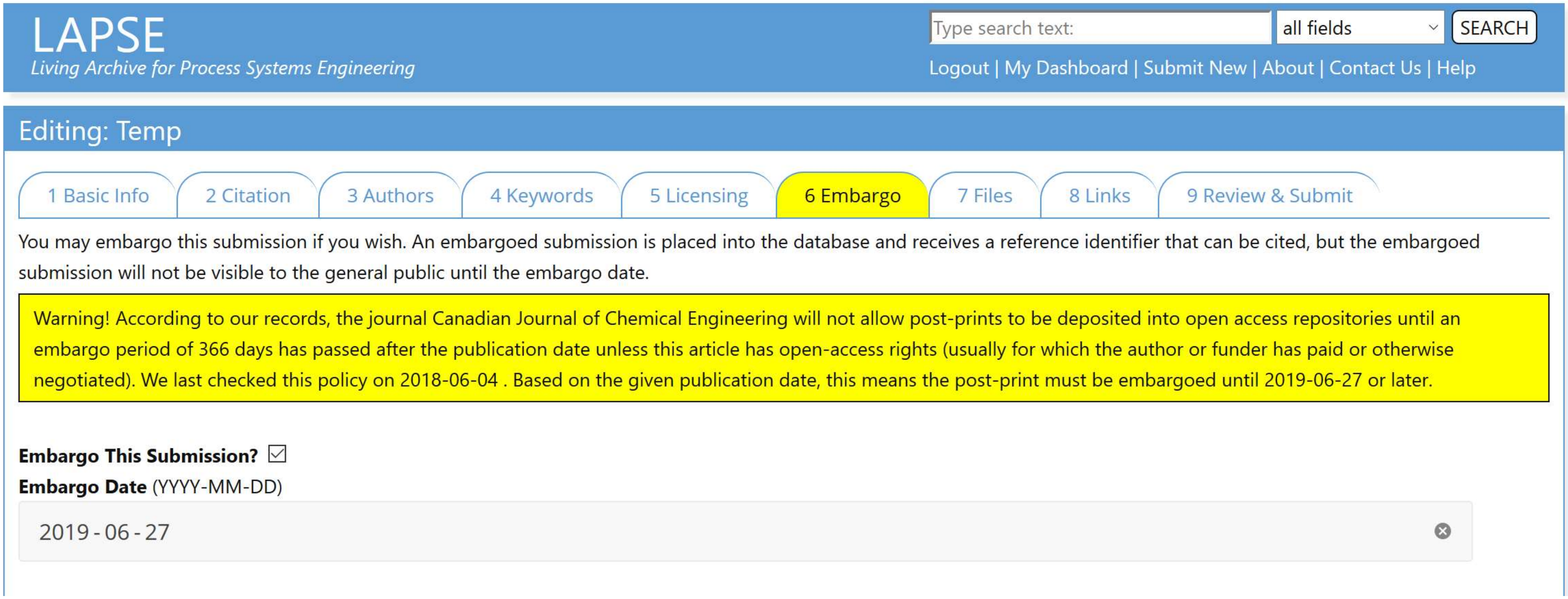

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A new approach to the identification of high-potential materials for cost-efficient membrane-based post-combustion CO2 capture

Authors:

Simon Roussanaly, Rahul Anantharaman, Karl Lindqvist, Brede Hagen

Date Submitted: 2018-06-22

Keywords: post-combustion, Attainable Region, property maps, gas separation membranes, CO2 capture

Abstract:

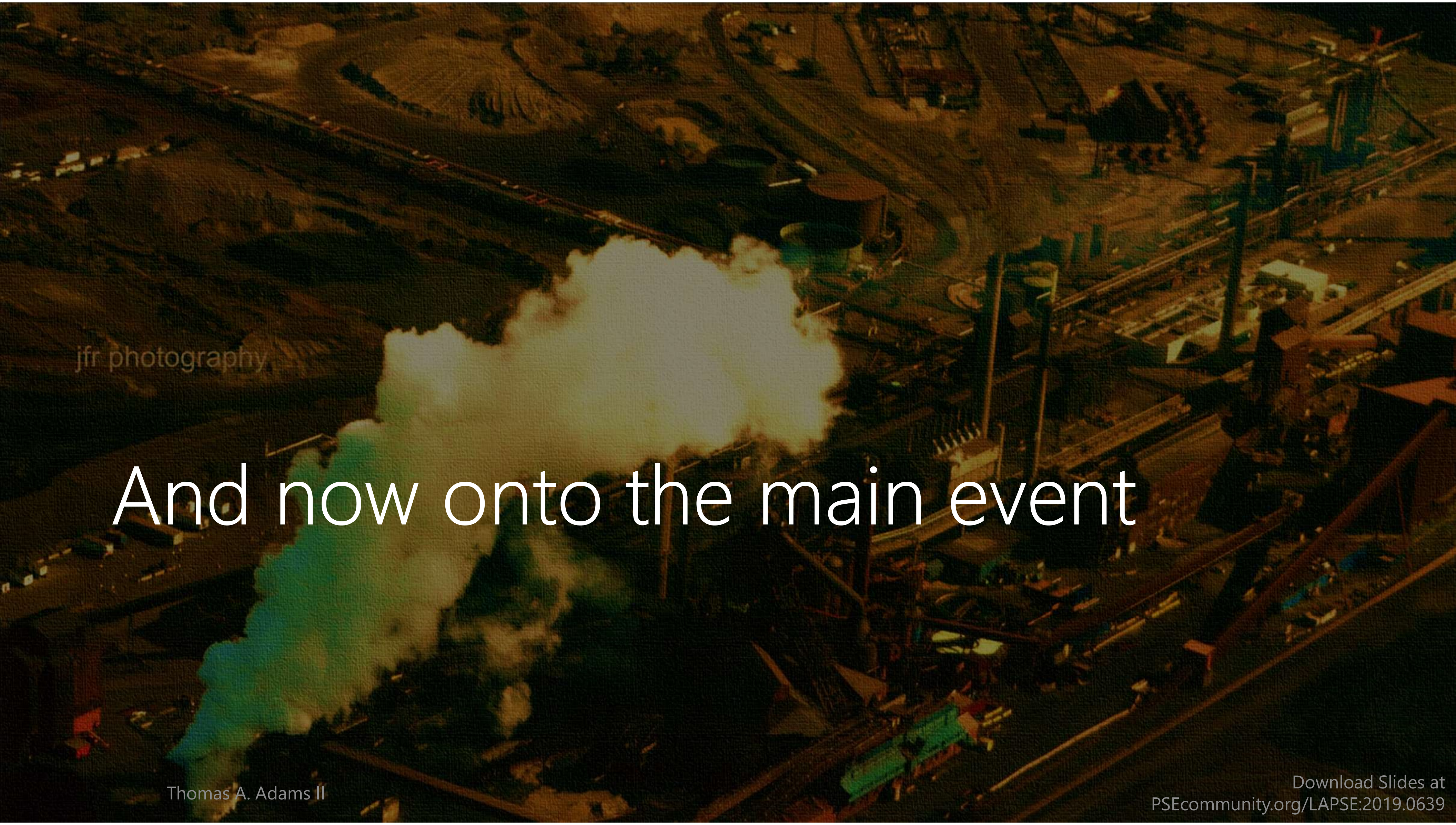
Developing “good” membrane modules and materials is a key step towards reducing the cost of membrane-based CO2 capture. While this is traditionally being done through incremental development of existing and new materials, this paper presents a new approach to identify membrane materials with a disruptive 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 Type: Published Article

Submitted To: LAPSE (Living Archive for Process Systems Engineering)

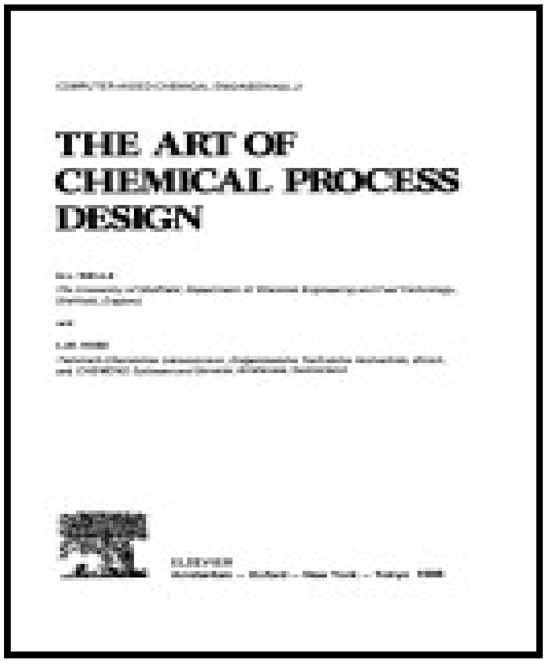
Citation (overall record, always the latest version):	LAPSE:2018.0142
Citation (this specific file, latest version):	LAPSE:2018.0142-1
Citation (this specific file, this version):	LAPSE:2018.0142-1v1

DOI of Published Version: https://doi.org/10.1039/C8SE00039E

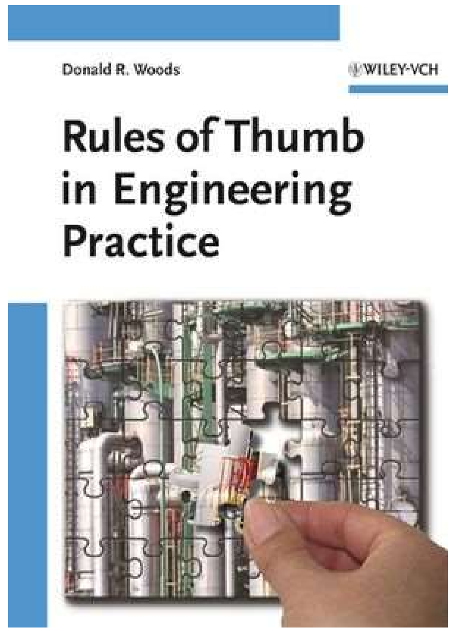


And now onto the main event

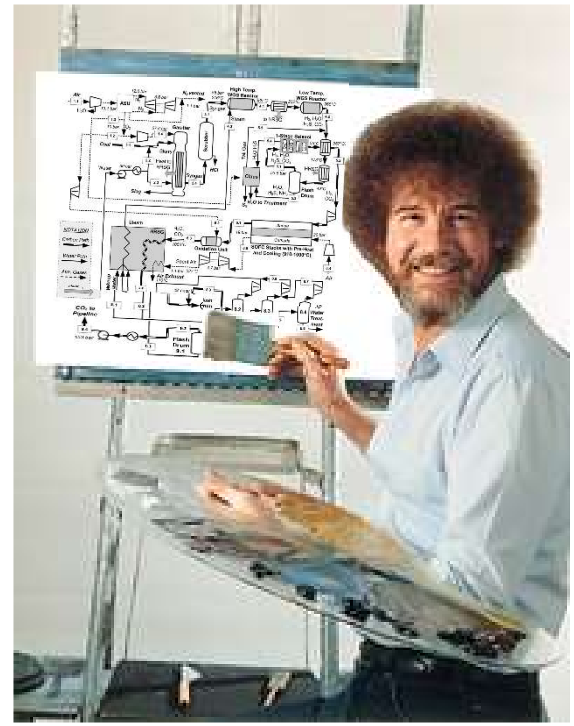
Process Design: Art and Engineering Merged



1986 Textbook by Wells and Rose (UK)



2007 Textbook by Don Woods (McMaster)



Identify the Artist by the Process?

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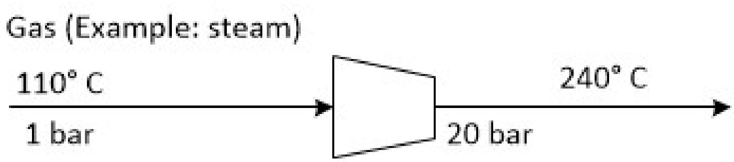
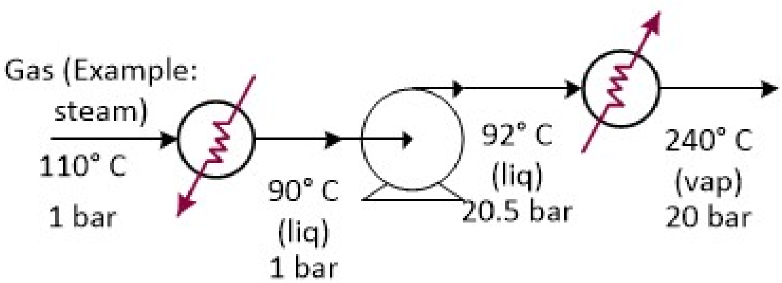
From Heuristics to Models

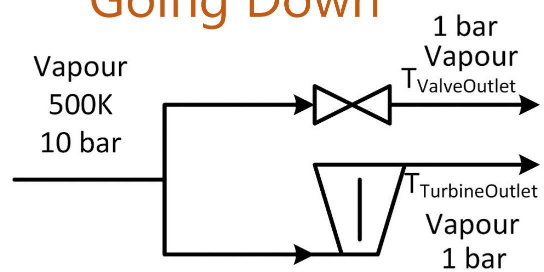
- Example question: Which is the *better* way of changing the gas pressure in these cases?

Going Up





Going Down



A) Use heuristics & engineering wisdom

B) Use simple first principles mathematical models by hand (e.g ideal gas law)

C) Use rigorous data driven / first principles mathematical models (e.g. Aspen Plus)

D) C inside eco-technoeconomic optimization framework within context of balance-of-plant

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Outcome goals for our Process Design Courses

Students should graduate with:

- a fundamental understanding of design concepts
- the ability to use the latest technologies and methods
- the ability to adapt, learn, and improve

Institutional expertise varies!

- Some departments have true experts
- Some professor experience mostly limited to own undergrad
- Some departments just hire from industry

We need different solutions for different situations

Future Trends in Process Design

Macro Trends (last 10 years): More Mathematical Modelling → Algorithms Replace Heuristic Decisions → Systems Analysis Thinking → Increased Complexity

Integration with Process control → Optimization (lots) → Product Design → Flexibility → Environment & Sustainability

New & Exciting Things Process Intensification → Mobile / Modular Tech. → Big Data → "Bigger" Software → Phenomena Level Design → Algorithmic flowsheet synthesis

- Big Data:
  - ANNs
  - Latent Variable Methods
  - PCA
- "Bigger" Software:
  - IDAES
  - Integration Suites
  - Aspen Energy Analyzer

Our students should get experience with these things

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Source: Martín M, Adams TA II. Future directions in process and product synthesis and design. *Comput. Chem. Eng.*, 128:421-436 (2019)

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Optimal Process Design Approaches

1: Locally(?) Optimize a Rigorous Model

Retain all the complexity of a flowsheet model

Simulation runs = black box objective function evaluation.

Still sequential modular

Derivative-free optimization or Black-box optimization

- Particle swarm, Genetic Algorithms, etc.
- Deterministic methods (Nelder-Mead)

2: Globally Optimize a Reduced Model

Reduced Complexity

- 0D / 1D models
- Made from more rigorous ones

May need to start from the full rigorous flowsheet model anyway

Equation-Oriented Framework

Mathematical MINLP programming techniques to solve

- incorporate risk

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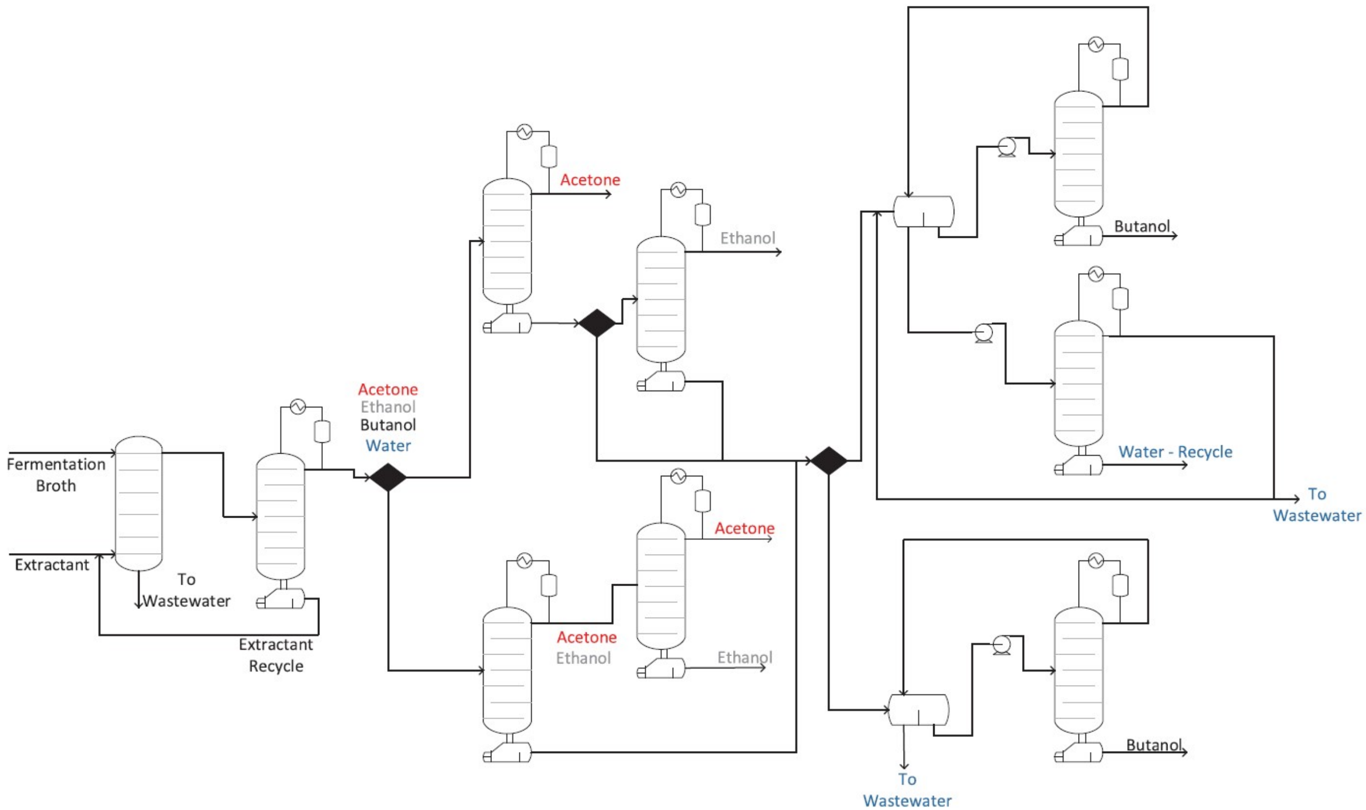
Flowsheet Optimization: Layout and Synthesis

- Superstructure Optimization
- Human designer lays out flowsheet of all possible options
- Optimal Flowsheet and unit design parameters chosen together



Source: Dalle Ave G, Adams TA II. Energy Conversion and Management 156 (2018) 288–300

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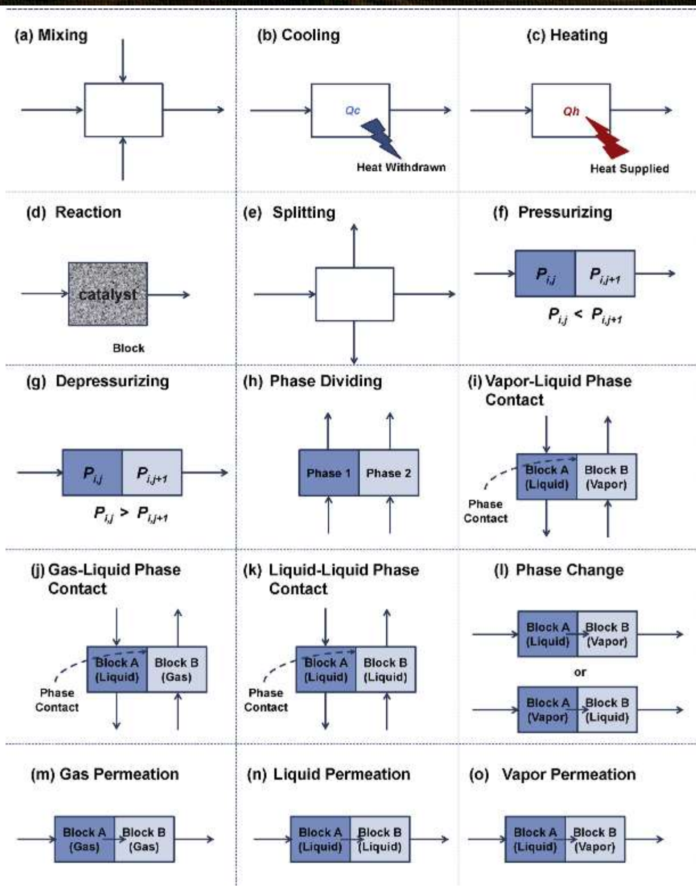
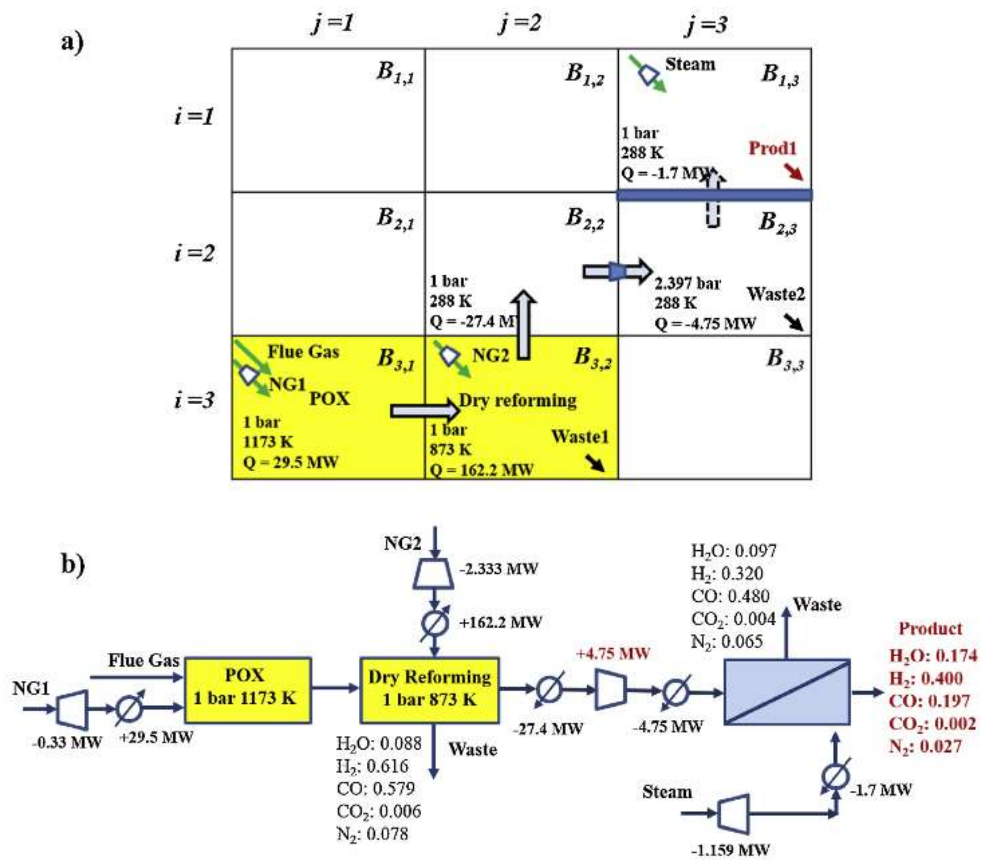
Innovative Approaches: Phenomena Level





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Source: S.E.Demireletal. / Computers and Chemical Engineering 105 (2017) 2–38

The Fundamental Skill in Which All are Linked

MATHERMATICAL MODELLING

At all levels

McMaster Approach – Modelling from Day 1

2nd year, Term 1
- Mass & Energy Bal's I
- Numerical Methods & Models

2nd year, Term 2
- Mass & Energy Bal's II & Thermo Lite
- Fluid Flow

3rd year, Term 1
- Separations
- More Thermo
- Heat Transfer
- Statistics & Latent Variable Methods

3rd year, Term 2
- Reactor Design
- Process Control
- Conceptual Process Design. Aspen

4th year, Term 1
- Advanced Reactors
- Advanced Separations
- Digital Process Control
- Energy Systems Engineering
- Economics, Operability, Safety

4th year, Term 2
- Process Optimization
- Big Data Models. MV Stats. PCA, PLS, ANN
- "Process Design"

Ways to integrate: Algorithmic thinking

2nd year, Term 1

- Mass & Energy Bal's I
- Numerical Methods & Models

2nd year, Term 2

- Mass & Energy Bal's II & Thermo Lite
- Fluid Flow

Macro Trends (last 10 years): More Mathematical Modelling → Algorithms Replace Heuristic Decisions

Provide tools for algorithmic solution early

- Matlab, Excel solvers
- Programming Skills

Avoid green engineering paper solutions

- Real problems aren't so conveniently defined
- Analytical solution rarely possible in practice

CACHE
Computer Aids for Chemical Engineering

Ideas for CAChE: Make it easy for the rest of your department to embrace systems thinking

- Tutorials / books (i.e. self-guided computer labs) for:
  - Numerical methods with Excel and Matlab
  - Optimization (easy stuff in Excel)
  - Problems designed to be used across the 3-4 year curriculum

Ways to Integrate: Data driven modeling

New & Exciting Things

Big Data Approaches

ANNs

Latent Variable Methods

PCA

Teaches first principles and first principles modeling

Revisit same ideas but with statistical and data-driven models.

- Revisit most critical fundamental chem eng principles
- High student demand

3rd year, Term 1

Separations

More Thermo

Heat Transfer

Statistics & Latent Variable Methods

CACHE
Computer Aids for Chemical Engineering

Ideas for CAChE:

- Big need for MOOC / modular lectures / tutorials / examples for data-based modeling
  - Something for integration into these common courses
- Example: Thermo: don't give them empirical equations of state or heat capacity curves. Make them create their own regression models from empirical data.
- One very good MOOC by Kevin Dunn.

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Ways to integrate: Systems thinking

Integration with → Optimization (lots) → Environment & Sustainability

New & Exciting Things → "Bigger" Software → Algorithmic flowsheet synthesis

Now by this point, there's time to incorporate

- Optimal flowsheet variables (i.e. feeds, recycle ratios)
- Optimal individual unit parameters in the systems context
- Superstructure optimization decision making
- Life cycle analysis

- (This is my course)

3rd year, Term 2

- Reactor Design
- Process Control
- Conceptual Process Design. Aspen

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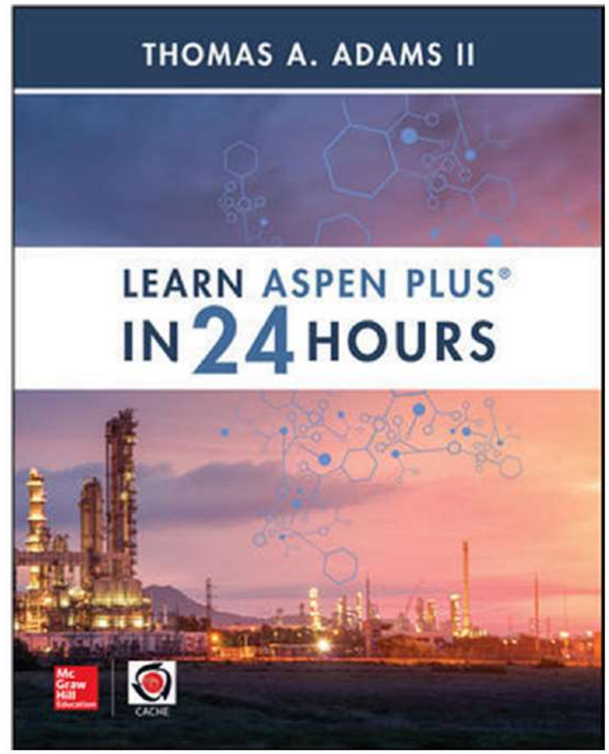
Computer Aids for Chemical Engineering



Design Course #2

Macro Trends (last 10 years): Systems Analysis Thinking → Increased Complexity

4th year, Term 1

Advanced Reactors

Advanced Separations

Digital Process Control

Energy Systems Engineering

Economics, Operability, Safety

Energy Systems Engineering [elective]

- Can focus on energy systems details since all students have process training already
- Students design large-scale energy systems (6 million population)
- Uses PSE methods and thinking
- (my course)

Second Design Course Incorporates

- Engineering Economics (cash flow, etc)
- Process Safety
- Operability
- Troubleshooting
- Scheduling
- Superstructure Optimization
- Flexibility / Flexible Designs

Final Design Course

New & Exciting Things → Process Intensification → Mobile / Modular Technologies → Big Data Approaches

The traditional capstone course

- Industrial, open ended problems
- Industrial mentors
- Students may incorporate GAMS / big data approaches from parallel courses
- Already have all technical skills, students strictly focus on defining & solving.
- Students choose their theme based on their specialty:
  - Water/Energy Technology
  - PSE
  - Biochem/Biomed
  - Polymers
- Most common student complaint is its "too easy"
- I wish this had more process intensification or "special" things

4th year, Term 2

Process Optimization

Big Data Models. MV Stats. PCA, PLS, ANN

"Process Design"

My Big Picture Vision

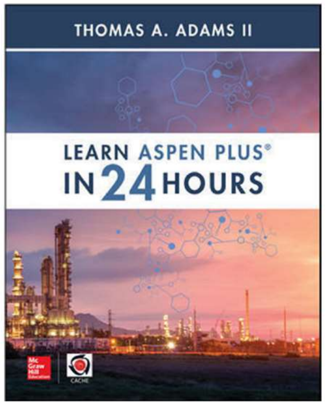
- Major parts of the curriculum trains:
  - Modelling
  - Algorithmic Thinking
- Unit Ops courses are updated:
  - Process Intensification
    - Reactive Distillation
    - Dividing Wall Columns, etc
  - Modular / Small Systems
  - Get rid of McCabe-Thiele / Underwood / Edmister (yeah I said it!!!)

- Design Sequence now has time for:
  - One classic chemical plant project
  - One "advanced" thing outside of this
    - Modular / Small
    - Bio
    - Pharma
    - Energy Systems (heat, storage, etc)

Recommendations for CAChE

Lessons from my book:

- Non-expert profs #1 market
- Designed for single-course but also cross-curriculum cherry-pick
- People switched their courses to Aspen Plus just because the book was available
- 12 x 2hr experiential learning tutorials
- Problem solving focus



CAChE Could Therefore:

- Fund more books like this
- Cross-cutting modules in different areas
- Focus on modelling
  - First principles
  - Data-driven
- Experiential Learning
- Algorithmic Thinking
  - As way of problem solving

Example Tutorials CAChE could fund

Thermo

- Provide experimental data
- Data-driven methods to make own make own models (example, find own Antoine's coeffs)

Distillation

- MESH equation approach instead of McCabe-Theile
- Build and solve own models!

Unit Ops

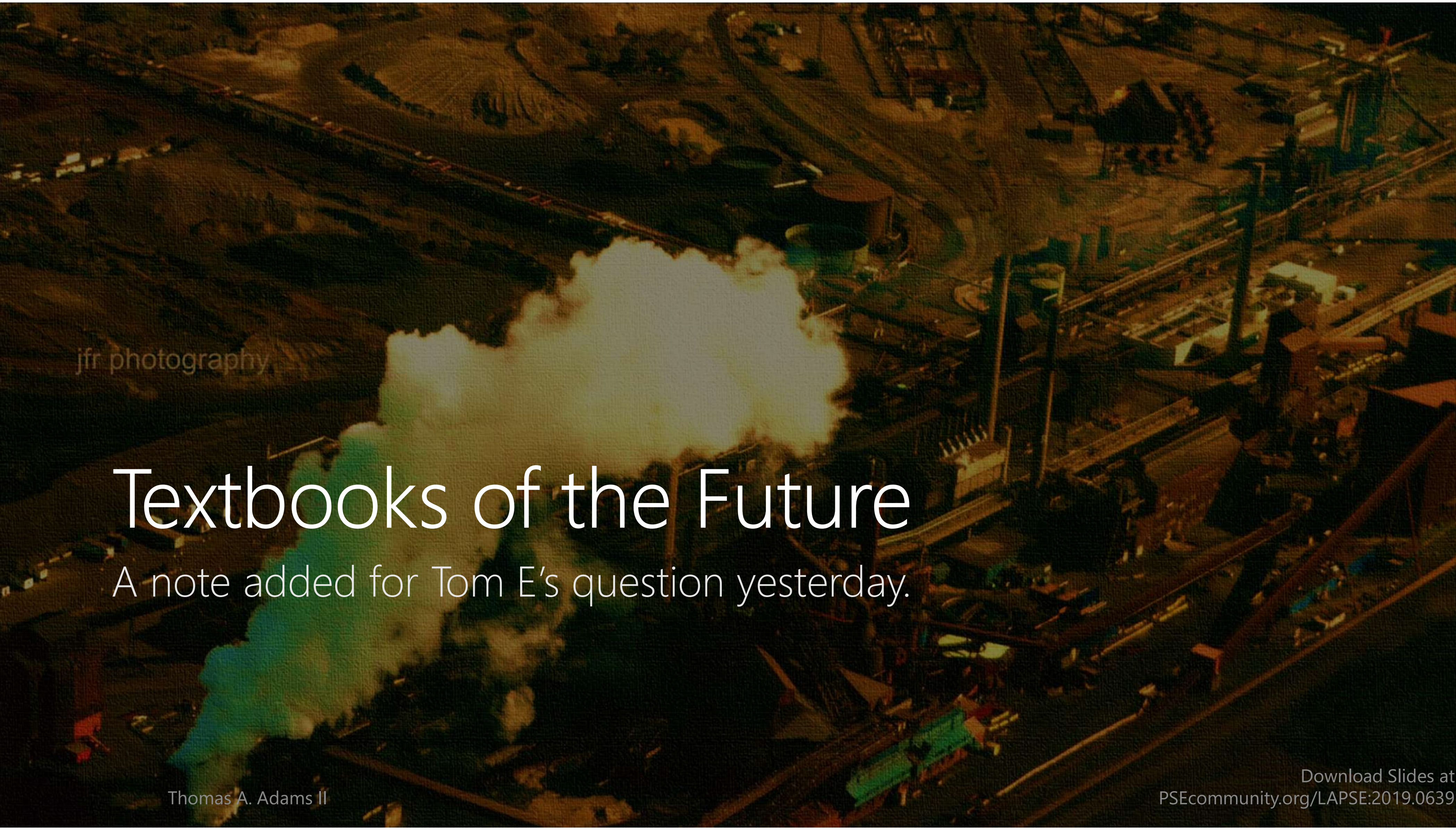
- Each student teams make a model for their own unit op
- First principles or data-driven
- Class links together to make one big flowsheet to solve a problem

Heat Transfer

- Regression of data to make curves for tube/shell pass correlations, FT,
- Shell balance model for simple heat exchanger

After many FOCAPD/CAChE-50 discussions:

- Movement toward less credits
  - Adding more courses not possible
- Process design experts unlikely to require/accept outside help
  - These are not the ones to worry about
  - PSE-research-heavy institutions are already at the leading edge
- It's the non-expert teachers who could use teaching materials
- The people that know about CAChE and the materials on the website are the least likely to need it.
  - Create different materials targeted at them.
- To make design better, integrate modelling and algorithmic thinking into everything else
- Frees up design course time to focus on more advanced, newer stuff
- Play to your strengths. Each institution is different for a reason.



Textbooks of the Future

A note added for Tom E’s question yesterday.

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My recent experience with my book

- PDF of book was on Facebook a few days *before* it was published.
  - Half of my royalties come from subscription-based HTML version
  - E-book (Kindle, etc) least popular
  - Students like hard copy (course is open-book)
- Books still carry reputation and trust
- But I think the institution subscription service is the way of the future. Netflix of textbooks.