

Modernizing the Undergraduate Process Design Curriculum

Recommendations for CAChE and everyone else

jfr photography



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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


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

CAChE Funded Venture



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LAPSE:2018.1189

McMaster University Course Lectures in Energy Systems Engineering

Thomas Alan Adams II

December 17, 2018

Lecture slides from the Fall 2018 CHEM ENG 4A03/6A03 Energy System Engineering course at McMaster University are attached. Energy Systems Engineering is a survey course that discusses many ways in which energy products are produced, transported, converted, and consumed in our society today. The lectures correspond to two 50-minute lectures a week for 13 weeks (some slide decks take 2 or 3 lectures to complete). The course cannot cover all energy systems of course, but focus mostly on large-scale or common processes either in use today or currently in development and research. The course takes a chemical engineering perspective so more attention is paid to processes and thermochemical phenomena and less attention is paid to issues related to mechanical engineering or electrical engineering, although there is some intersection.

The lecture slides include the following topics:

- 1.1. Life Cycle Analysis (basic review)
- 1.2. Key Metrics in Energy Systems
- 2.1. Coal Production
- 2.2. Natural Gas Production
- 2.3. Biomass Harvesting
- 2.4. Petroleum Production
- 3.1. Pulverized Coal Power Plants
- 3.2. Natural Gas Power Plants
- 3.3. Nuclear Power Plants
- 3.4. Solar Energy
- 3.5. Wind Energy
- 4.1. Gasification and IGCC
- 4.2. CO₂ Capture and Sequestration
- 4.3. Oxyfuel Combustion
- 4.4. Chemical Looping Combustion
- 4.5. Fuel Cells
- 5.1. Petroleum Refining
- 5.2. Biofuels
- 5.3. Synthetic Transportation Fuels (including Fischer-Tropsch)
- 5.4. Alternative Transportation Fuels
- 6.1. District Energy

All content was created by Thomas A. Adams II, except for Nina Silva Montiero who made Lecture 6.1. The course does not have one specific textbook associated with it but instead draws from a wide variety of books, reports, journal articles, and government sources. Citations are given at the bottom of each individual slide.

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1. LAPSE:2019.0638

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 Abasaed, 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... [\[more\]](#)

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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

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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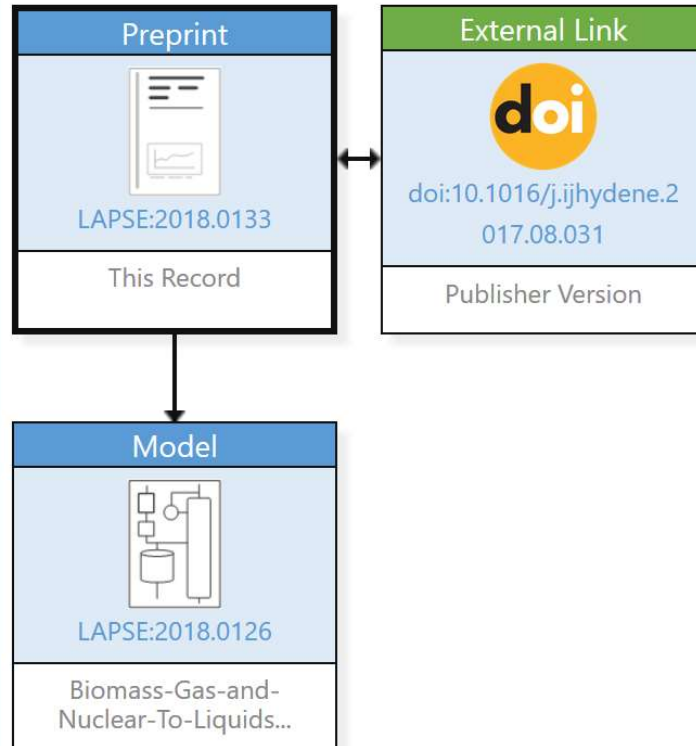
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Published Version [\[10.1016/j.ijhydene.2017.08.031\]](#)

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Create Research Map

- Give big picture overview of your research program
- Tree of how each work relates to the rest
- Ex: Connect conference presentations to corresponding papers
- Connect to the work of others as well.
- Connect to educational materials

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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.

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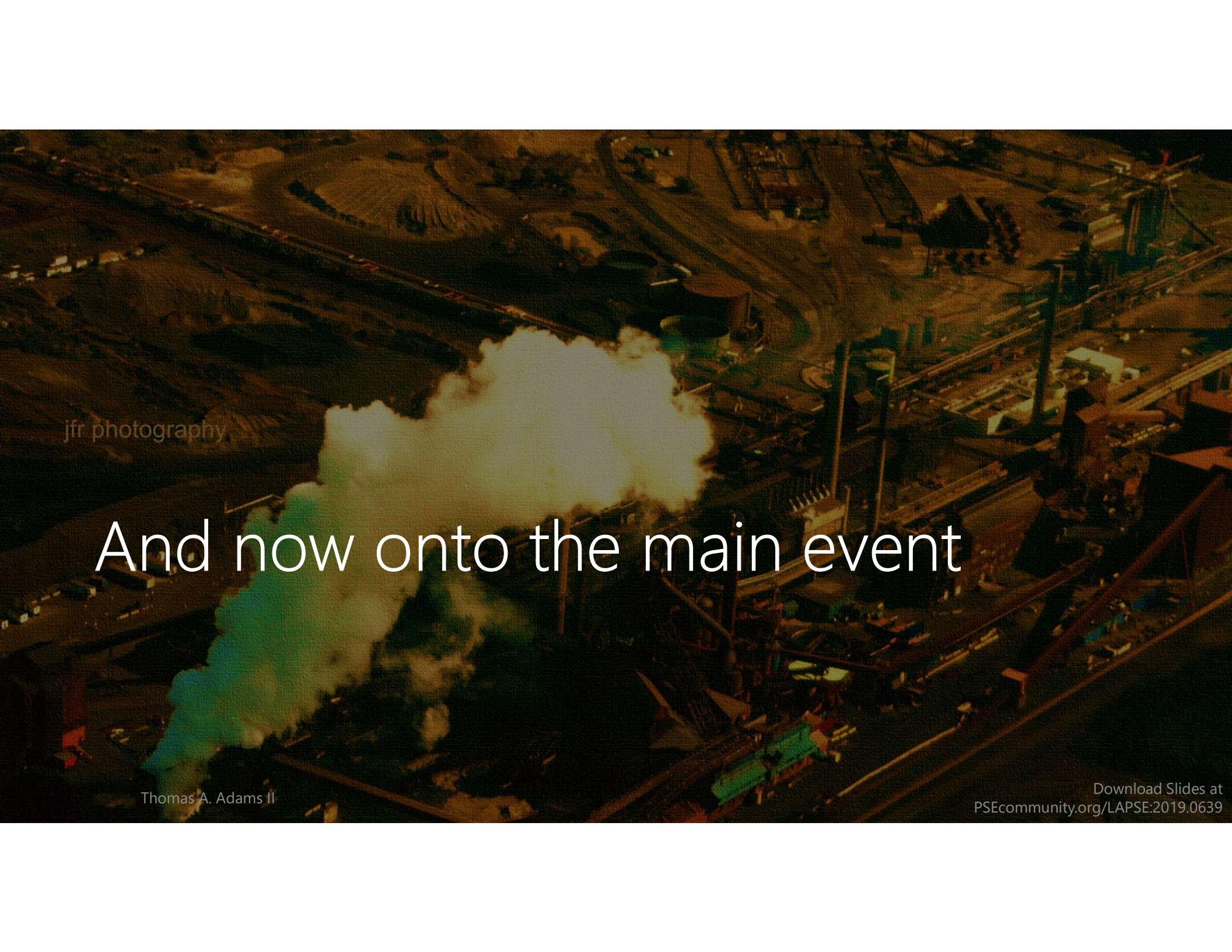
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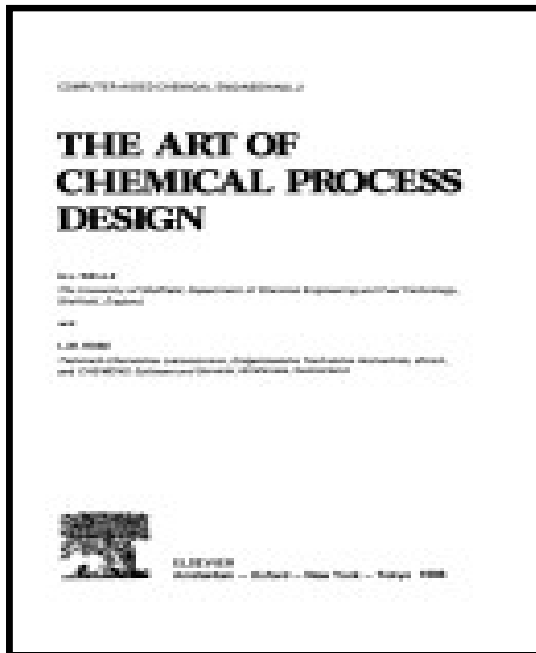
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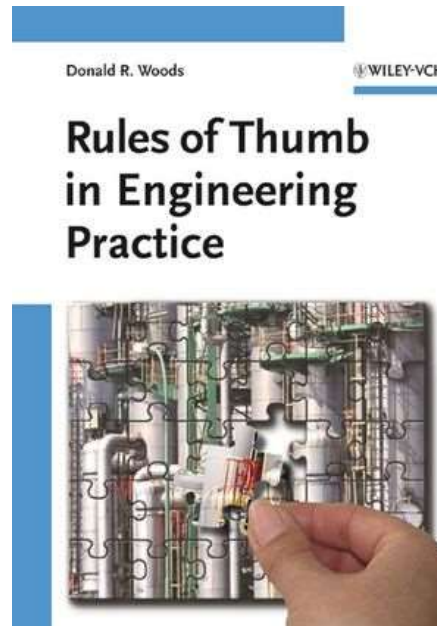
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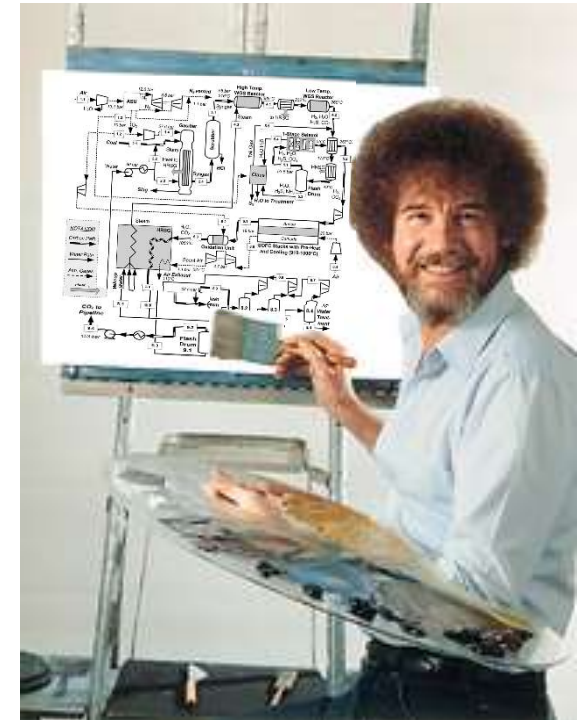
Process Design: Art and Engineering Merged



1986 Textbook by
Wells and Rose (UK)



2007 Textbook by
Don Woods
(McMaster)

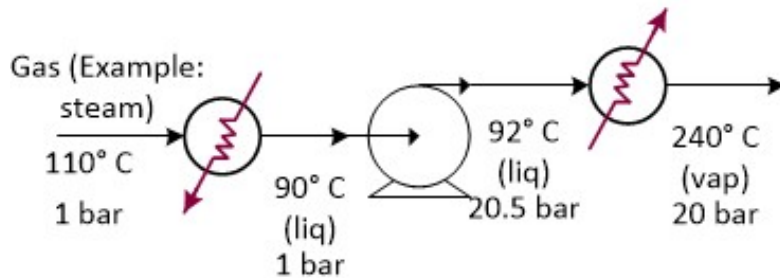
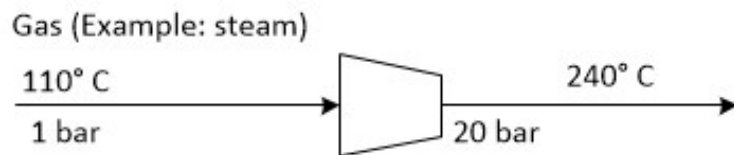


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Process?

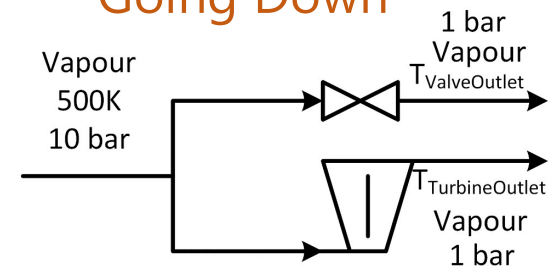
From Heuristics to Models

- **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

Outcome goals for our Process Design Courses

Students
should
graduate with:

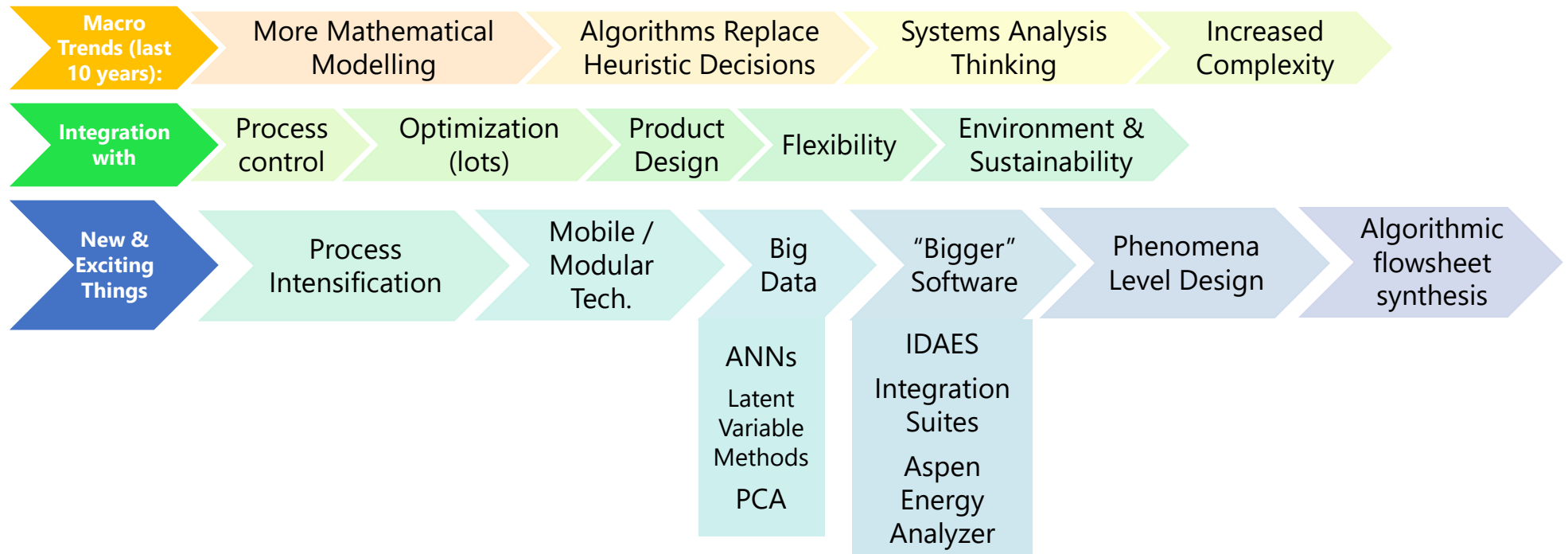
- a fundamental understanding of design concepts
- the ability to use the latest technologies and methods
- the ability to adapt, learn, and improve

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

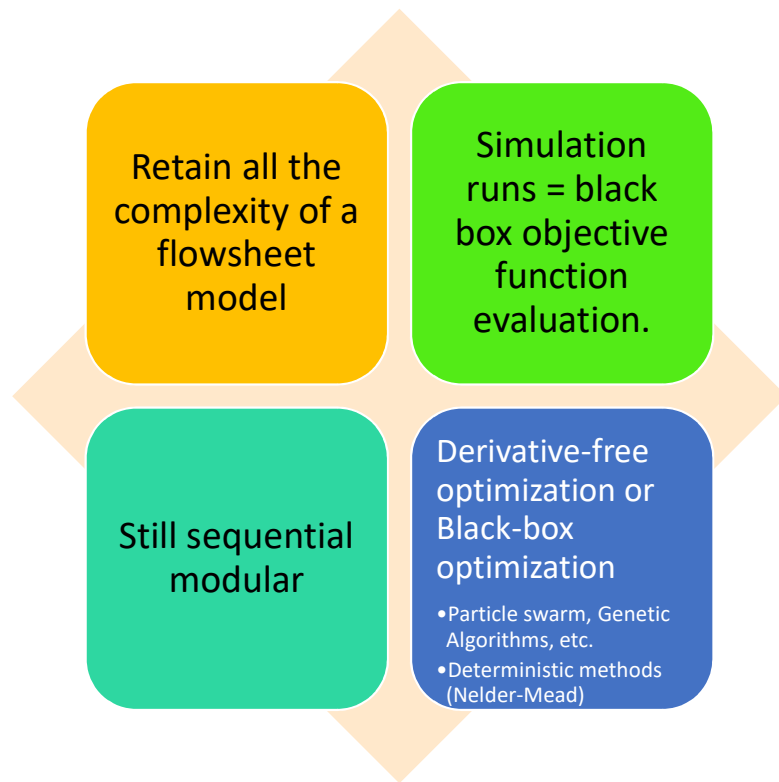
Future Trends in Process Design



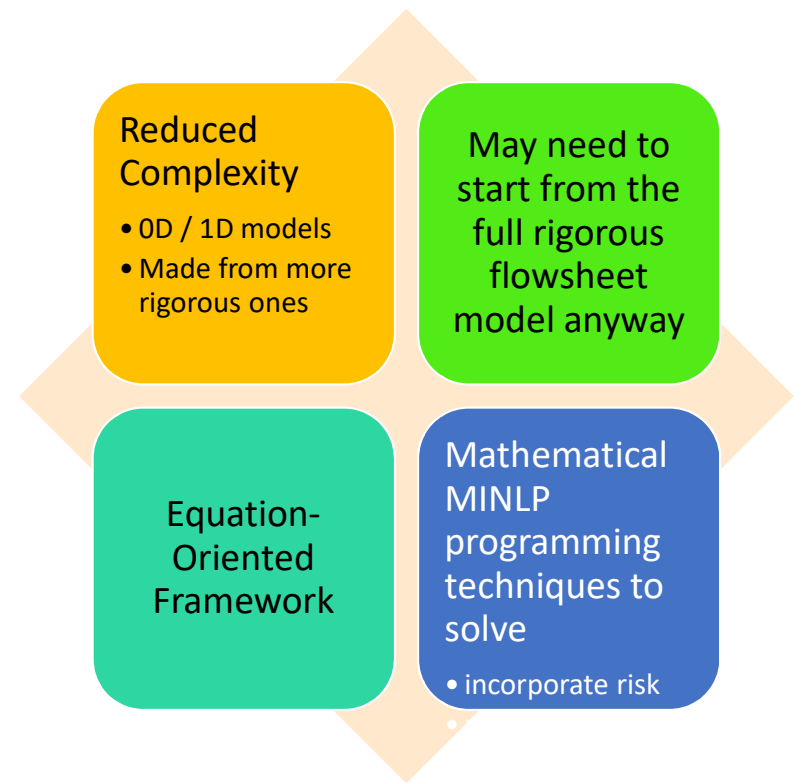
Our students should get experience with these things

Optimal Process Design Approaches

1: Locally(?) Optimize a Rigorous Model

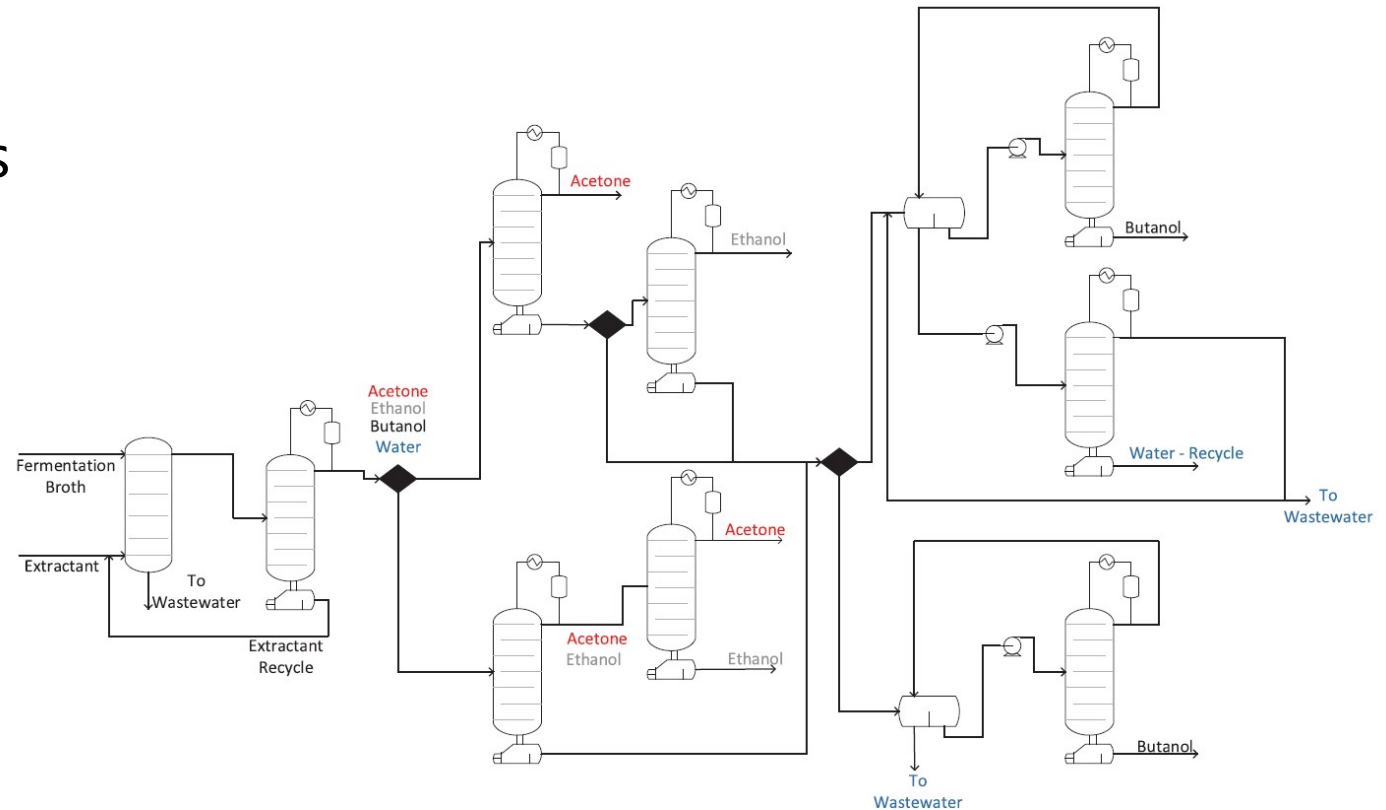


2: Globally Optimize a Reduced Model

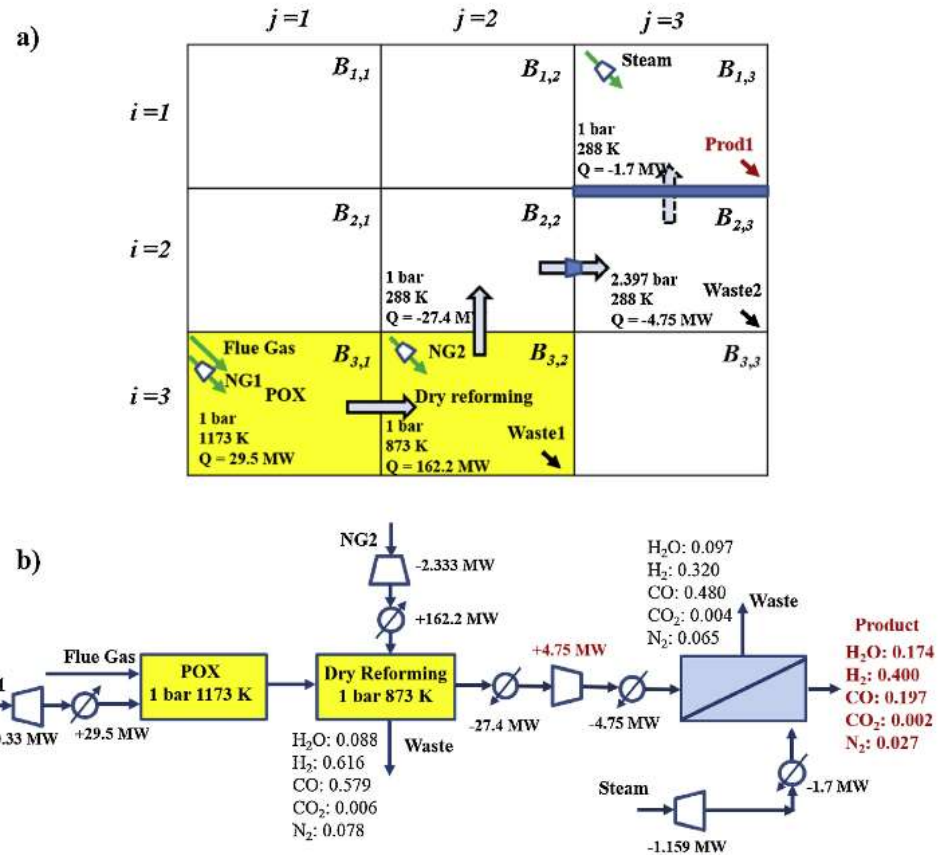
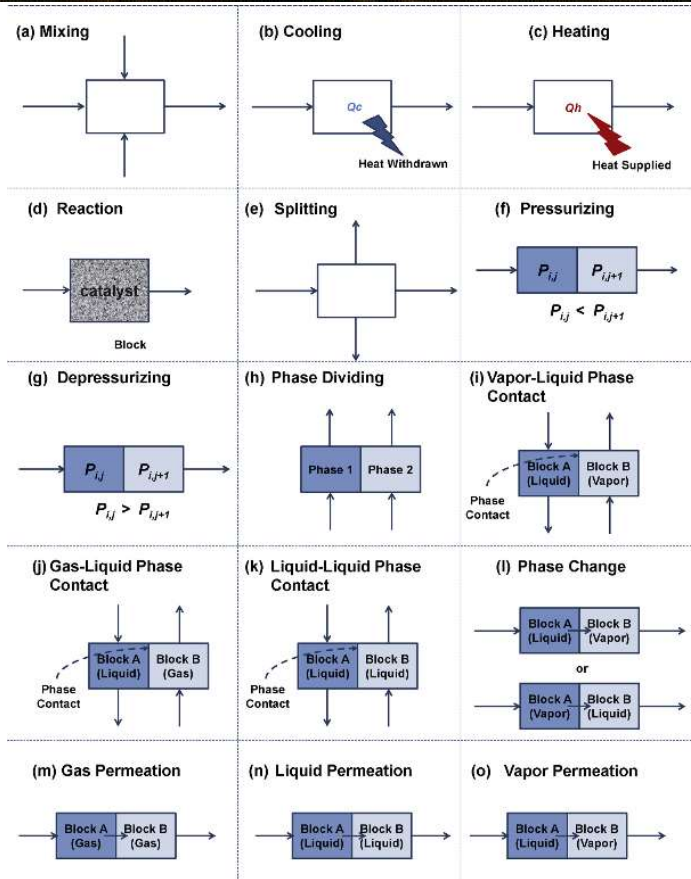


Flowsheet Optimization: Layout and Synthesis

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



Innovative Approaches: Phenomena Level



The Fundamental Skill in Which All are Linked

MATHEMATICAL 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

Provide tools for
algorithmic solution early

- Matlab, Excel solvers
- Programming Skills

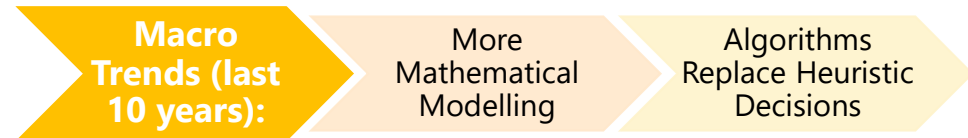
2nd year,
Term 2

Mass &
Energy Bal's
II & Thermo
Lite

Fluid Flow

Avoid green engineering
paper solutions

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

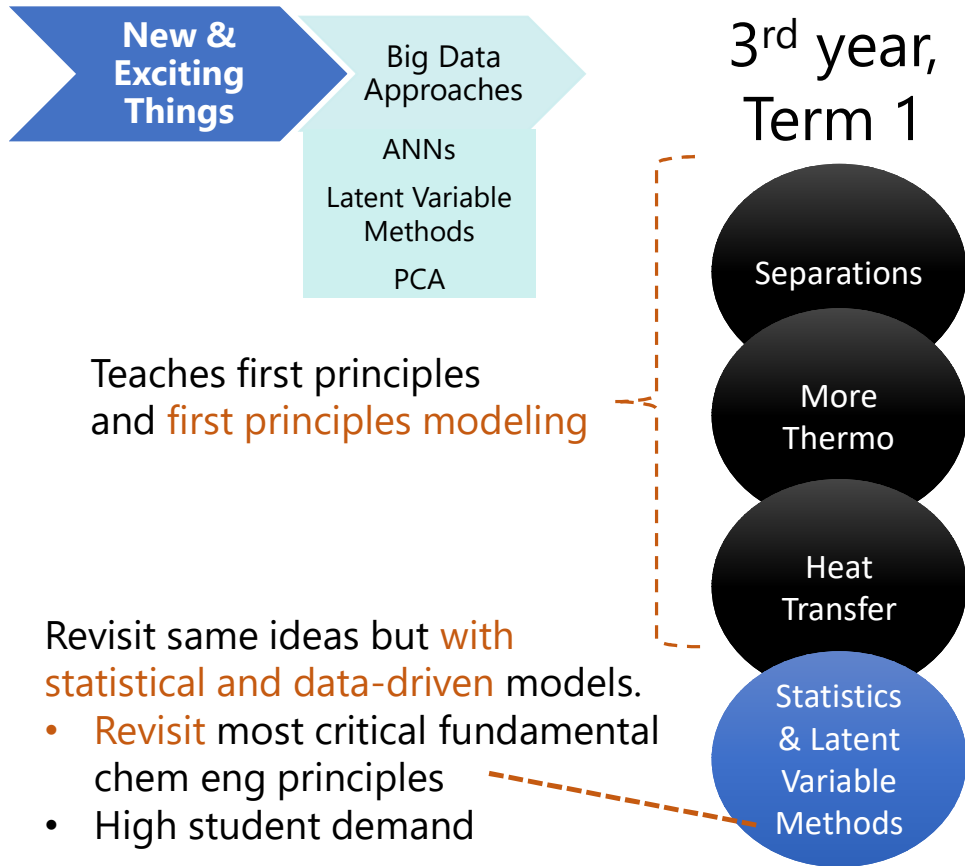


Computer Aids for Chemical Engineering

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

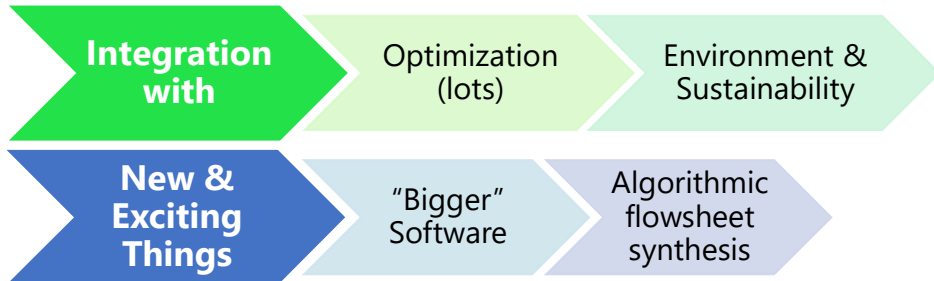


Computer Aids for Chemical Engineering

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.**

Ways to integrate: Systems thinking



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

 **CACHE**

Computer Aids for Chemical Engineering

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Design Course #2

Macro
Trends (last
10 years):

Systems
Analysis
Thinking

Increased
Complexity

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

4th year,
Term 1

Advanced
Reactors

Advanced
Separations

Digital
Process
Control

Energy
Systems
Engineering

Economics,
Operability,
Safety

Final Design Course



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”

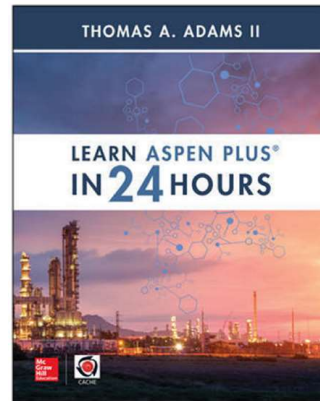
My Big Picture Vision

- 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 models (example, find own Antoine's coeffs)

Distillation

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

Unit Ops

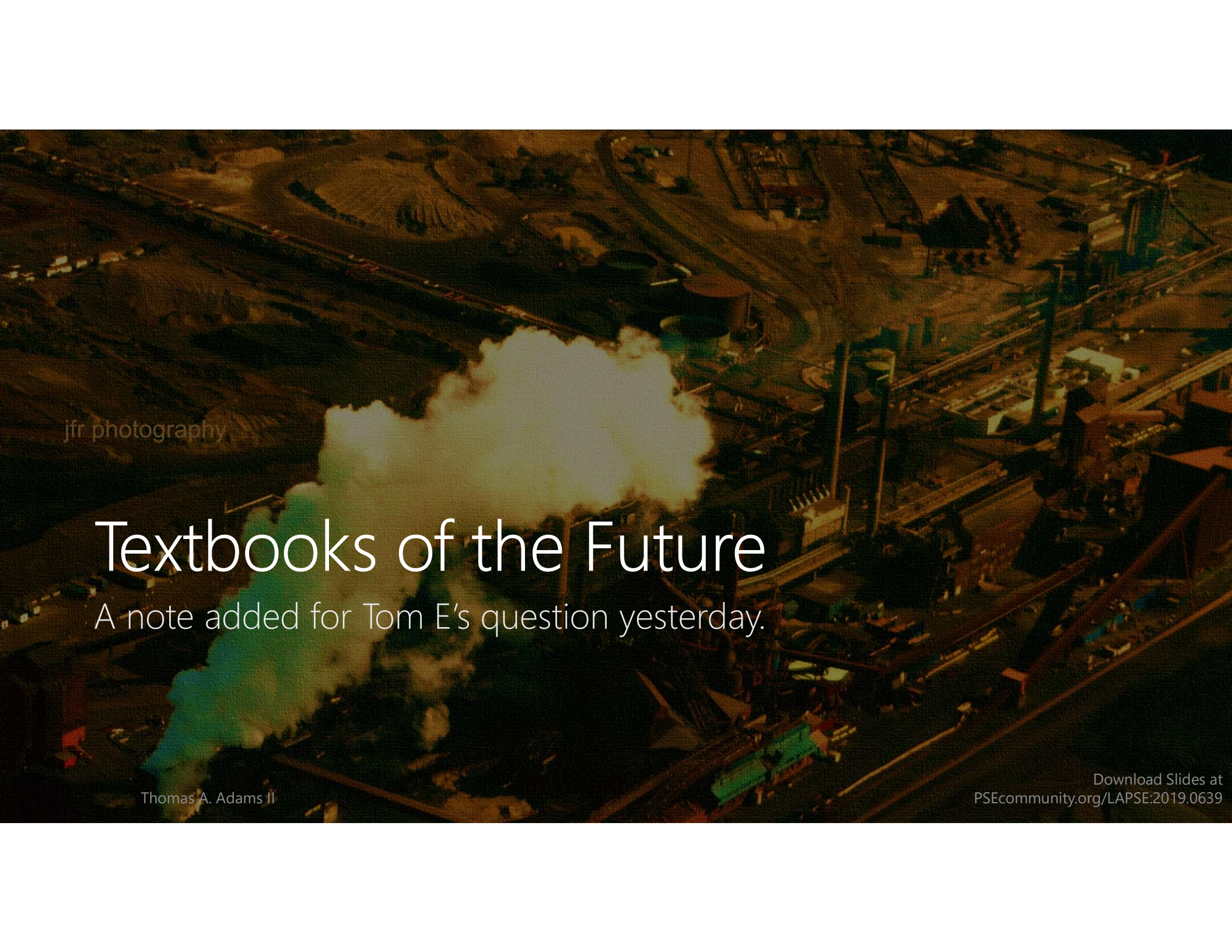
- Each student teams make a model for their own unit op
- First principles or data-driven
- Class links together to make one big flowsheet to solve a problem

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.

An aerial photograph of an industrial facility, possibly a refinery or chemical plant. The image shows a complex network of pipes, storage tanks, and buildings. A large, billowing plume of white smoke or steam rises from the center of the facility, partially obscuring some of the structures. The overall color palette is dominated by the greys and browns of the industrial infrastructure, with the bright white of the smoke providing a strong contrast.

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Textbooks of the Future

A note added for Tom E's question yesterday.

Thomas A. Adams II

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