IDAES

Institute for the Design of Advanced Energy Systems

2017 Crosscutting Research Project Review

March 21, 2017

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Institute for the Design of Advanced Energy Systems

- **Vison:**
  - Become the **premier resource for the identification, synthesis, optimization and analysis** of innovative advanced energy systems at scales ranging from process to system to market.
- **Challenges:**
  - Determining **which technologies to pursue** and **how to optimally integrate them** while taking into account their full life cycle environmental footprint and determining their potential in the market.
  - Current computational tools and analysis approaches cannot simultaneously address such complex interactions, nor can they address a sufficient number of scenarios in the timeframes required.
- **Integrates NETL's historic capabilities in Systems Engineering & Analysis**
  - Energy processes
  - Life cycle environmental impacts
  - Energy infrastructure
  - Energy markets
- **Impact:**
  - **Rapid integrated identification and assessment of novel energy technologies** and their potential impact within complex systems and markets in order to prioritize and direct R&D efforts.
  - **Actively assist development and scale-up** of advanced energy systems

Development Of Innovative Advanced Energy Systems Through Advanced Process Systems Engineering

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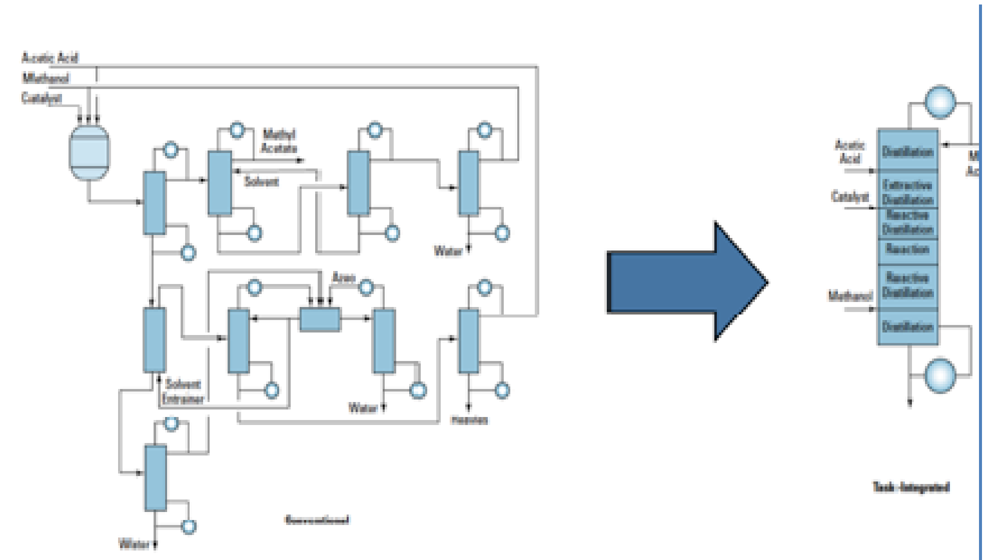
- **Approach:** Develop and utilize multi-scale, simulation-based computational tools and models to support design, analysis, optimization, scale-up and troubleshooting.
- **Next generation modeling and optimization platform**
  – Flexible and open modeling environment
  – Complete provenance information
  – Supports advanced solvers and computer architecture
  – Intrusive uncertainty quantification
  – Process synthesis, integration, and intensification
  – Process control and dynamics
- **Apply to development of new & novel energy systems**
  – Chemical Looping
  – Advanced Combustion Concepts
  – Transformational Carbon Capture



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IDAES Project Goals

- Demonstrate next generation capabilities for synthesizing optimized energy systems
  - **Actively assist development and scale-up:** Chemical looping, oxycombustion, and other advanced energy systems
  - **Flexible design approaches:** Optimization over broad ranges of potential plant operation (feeds, loads, etc)
  - **Semi-intrusive UQ:** Unprecedented understanding of technical and market risks
  - **Process intensification:** Step-change technologies that are smaller, more modular and more cost effective
  - **Advanced computing:** New algorithms to enable multicore, many core (GPU) and distributed computing for large scale optimization codes, particularly NLP and MINLP solvers
- Demonstrate a fully integrated framework for advanced process systems engineering
  - Modeling environment
  - Data management system
  - Semi-intrusive UQ
  - Global optimization
  - Process intensification
  - Distributed computing
- Demonstrate a fully integrated advanced multi-scale simulation toolset
  - Unified architecture to support the complete life cycle from concept to design, start-up and operation.

IDAES Modeling Framework

- **Based on Pyomo http://www.pyomo.org/**
  - Python-based general mathematical modeling language
  - From Sandia National Laboratory
  - Developers are integral to IDAES
  - Open-source
  - Interface to advanced optimization solvers
  - Automatic discretization of PDEs
  - **New:** DAE solver interface for dynamic modeling
- **Process modeling software environment**
  - Standards for process/property models
  - Inter-connectable flowsheet, unit and sub-models
  - Expedite development of process models
  - Load/save model states
  - Initialization

Task Structure

1. Project Management

2. Conceptual Design, Optimization, UQ, and Intensification of Advanced Energy Systems (NETL, CMU, WVU)

3. Software Architecture, Algorithms, and Distributed Computing (Sandia, LBL, CMU)

4. PSE Support for Advanced Combustion Systems (NETL)

   – Modeling to directly support internal and external ACS projects, including chemical looping

   – Working with program to explore collaboration with B&W, WUST, GTI

Example IDAES Workflows

High Fidelity Models	Smart Model Reduction Strategies	Equation Oriented Process Optimization	Results
Rigorous Unit Operation Models	Algebraic Surrogate Models e.g., ALAMO	Conceptual Design to Find Optimal Process Configuration	Optimized Process Configuration
Rigorous Kinetic and Thermodynamic Models	Cozad, Sahinidis, Miller, 2014, AIChE J.	Advanced Process Systems Optimization of Fixed Flowsheets	Optimized Process Conditions

Example IDAES Workflows

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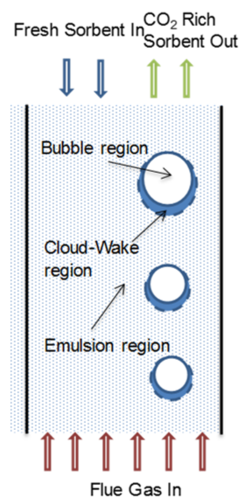
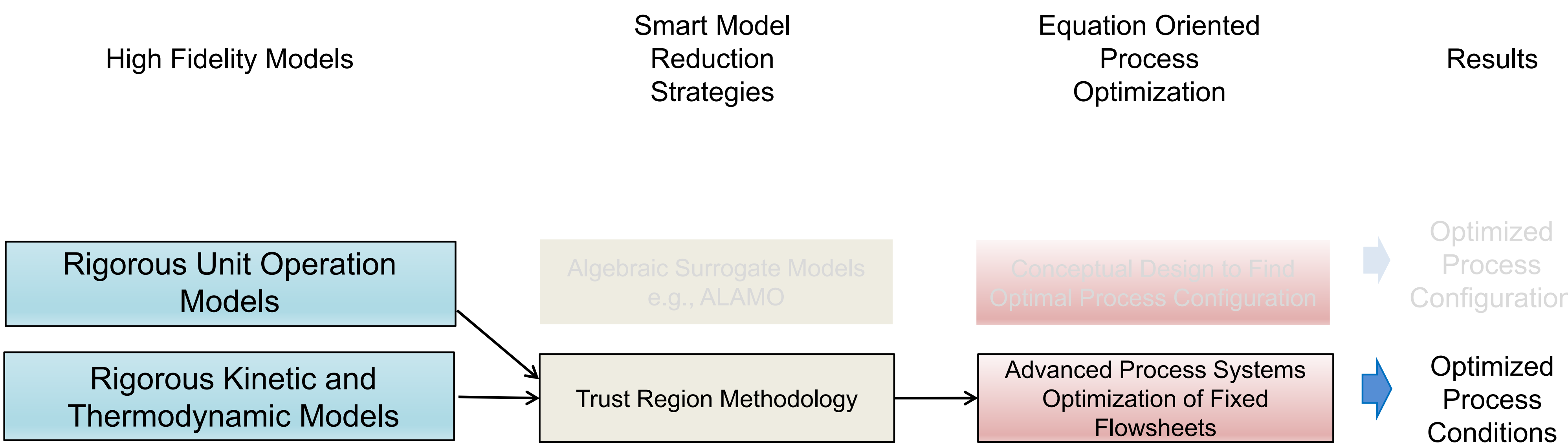


- Bubbling Fluidized Bed (BFB) for solid-sorbent based CO2 capture system
- 1-D, 3 region, non-isothermal, 6 components
- **14,187 Algebraic Equations** (1994 PDEs)

Lee and Miller, 2013, Ind. Eng. Chem. Res.

- **Surrogate model containing 8 "optimization friendly" algebraic equations**
- Outlet T, P, composition as a function of input conditions, equipment geometry

Advanced Oxycombustion Systems Optimization



<u>Application</u>:
Oxycombustion

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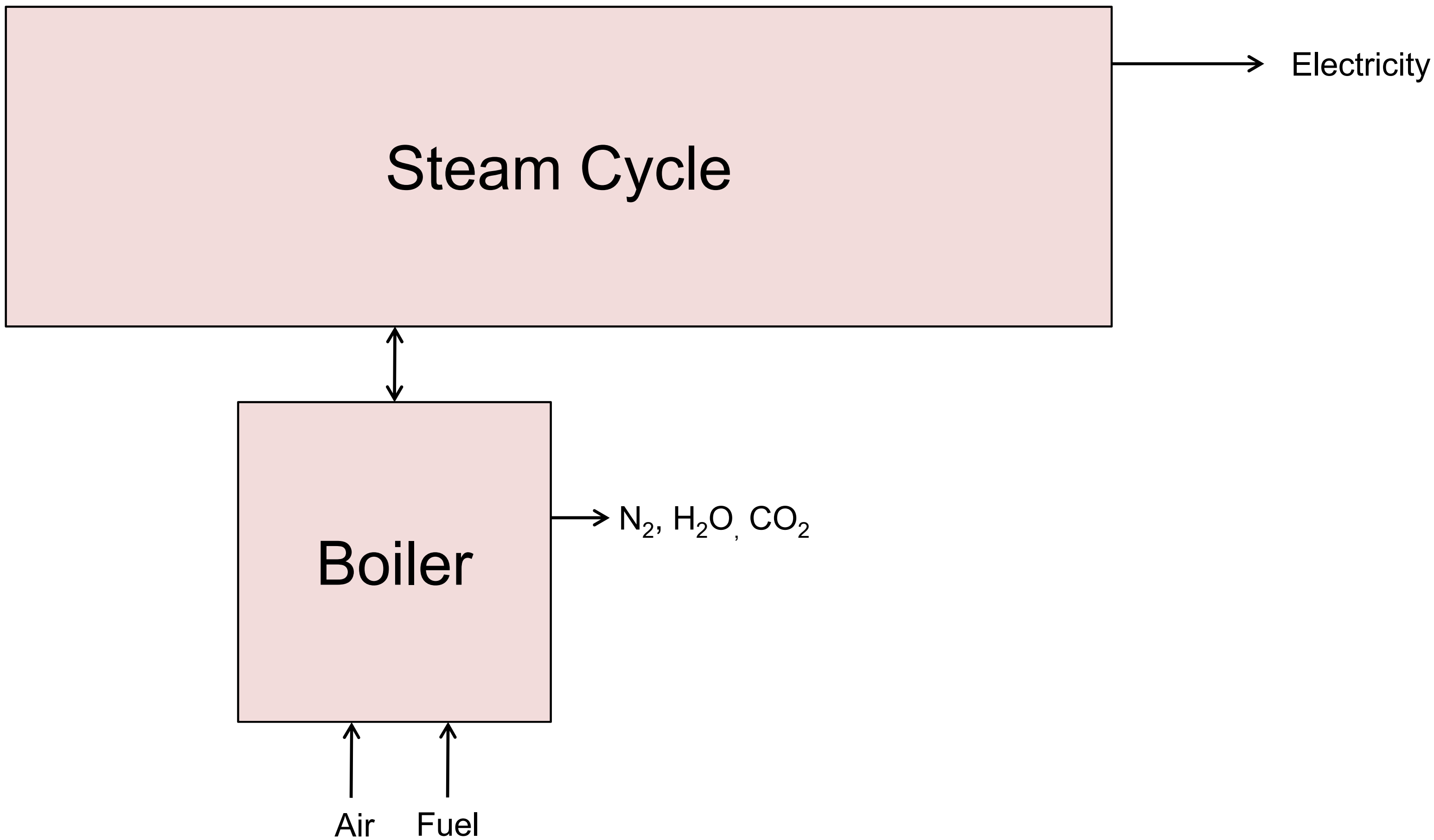
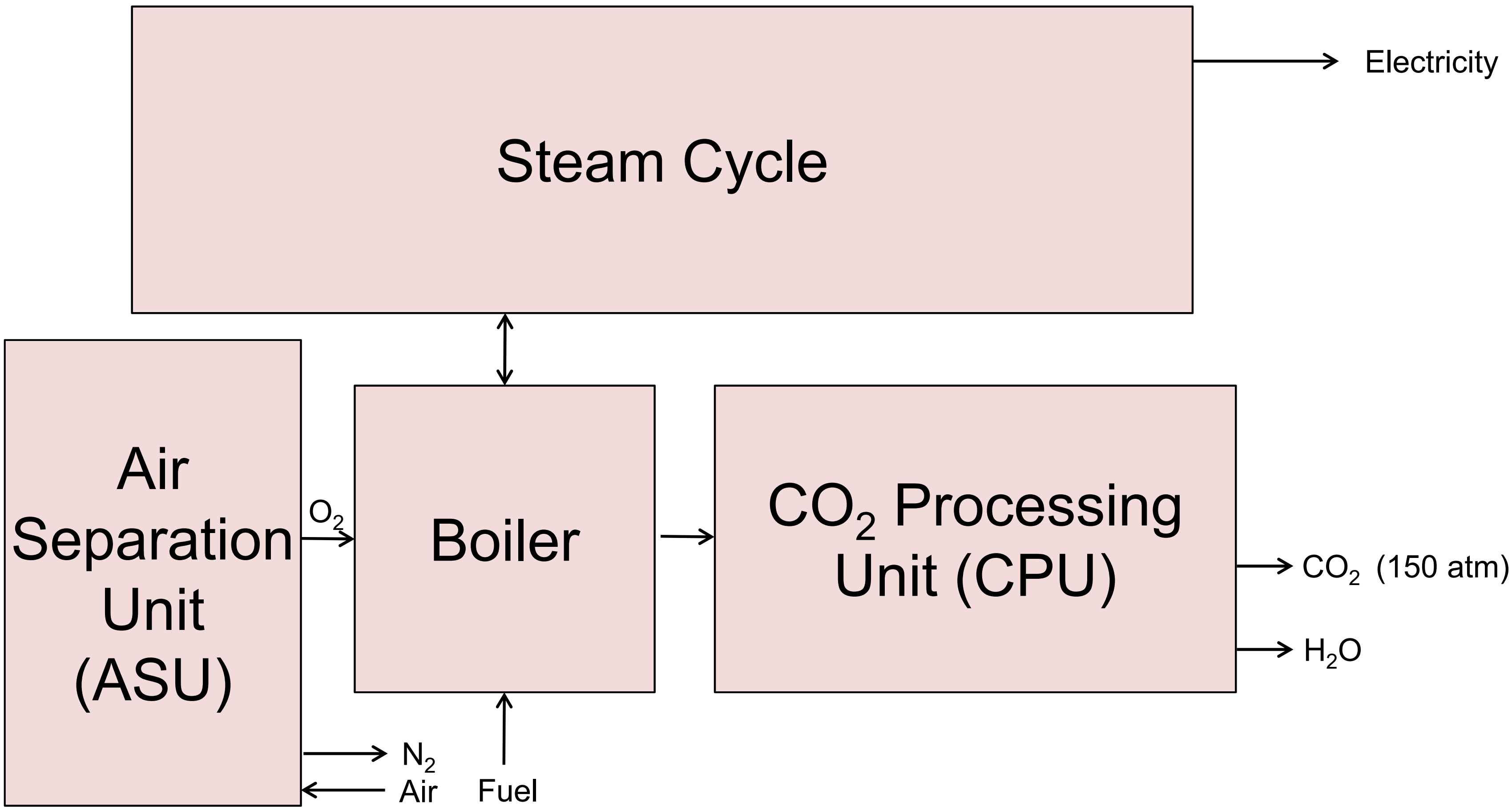
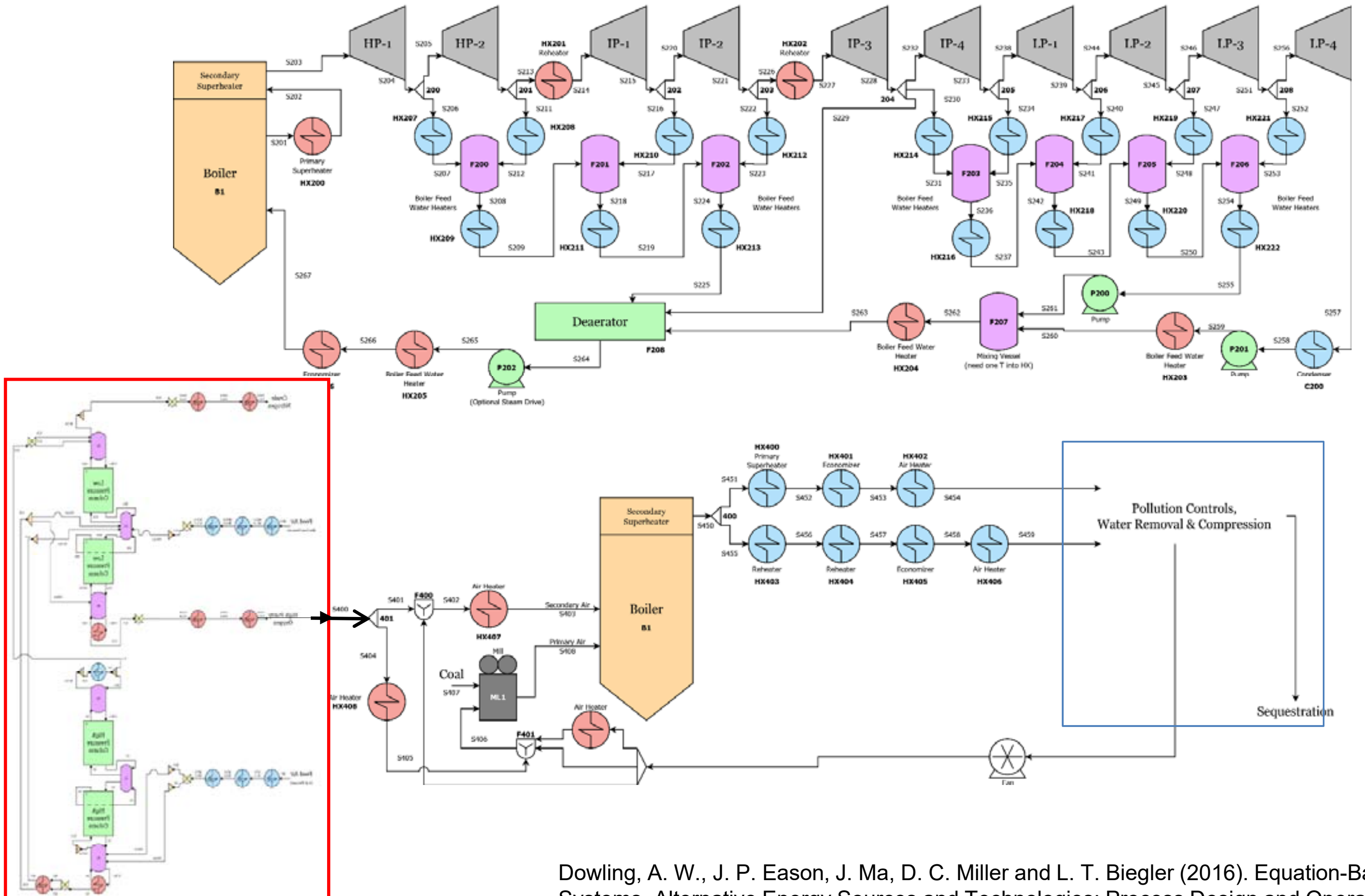
Traditional Coal-Fired Power Plant



Oxycombustion Power Plant



Advanced Oxycombustion Systems Optimization



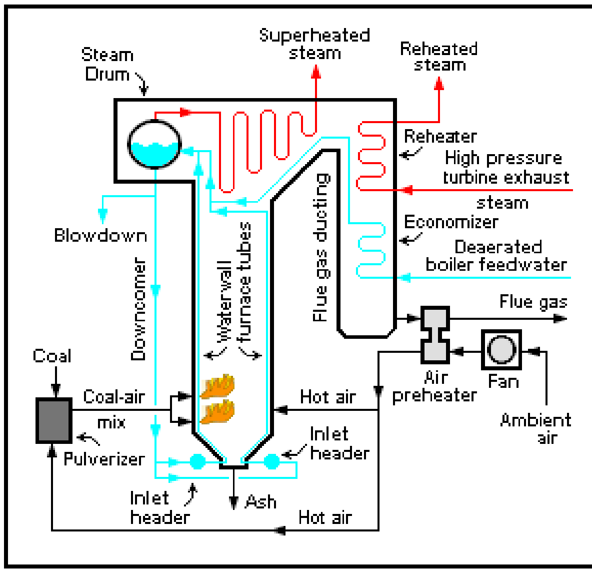
Min **Levelized Energy Cost**
s.t.
- Steam cycle connectivity
- Steam thermodynamics
- Heat exchanger models
- Pump model
- Turbine model
- Heat integration model
- ASU and CPU Models
- **Hybrid boiler model**

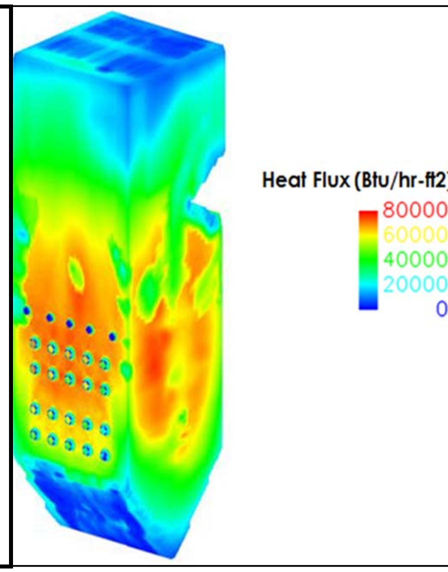
Dowling, A. W., J. P. Eason, J. Ma, D. C. Miller and L. T. Biegler (2016). Equation-Based Design, Integration, and Optimization of Oxycombustion Power Systems. Alternative Energy Sources and Technologies: Process Design and Operation. M. Martín. Cham, Springer International Publishing: 119-158.

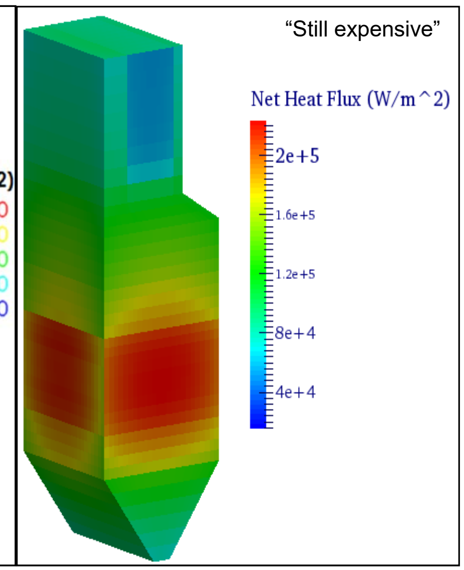
Integrating Detailed Boiler Model

Hybrid 1-D (char kinetics, flow)
3-D (radiative heat transfer):
2-3 minutes to solve

CFD model: 2-3 weeks to solve







Ma, J.; Eason, J. P.; Dowling, A. W.; Biegler, L. T.; Miller, D. C., Development of a First-Principles Hybrid Boiler Model for Oxy-Combustion Power Generation System. *International Journal of Green House Gas Control*, **2016**, 46, 136-157

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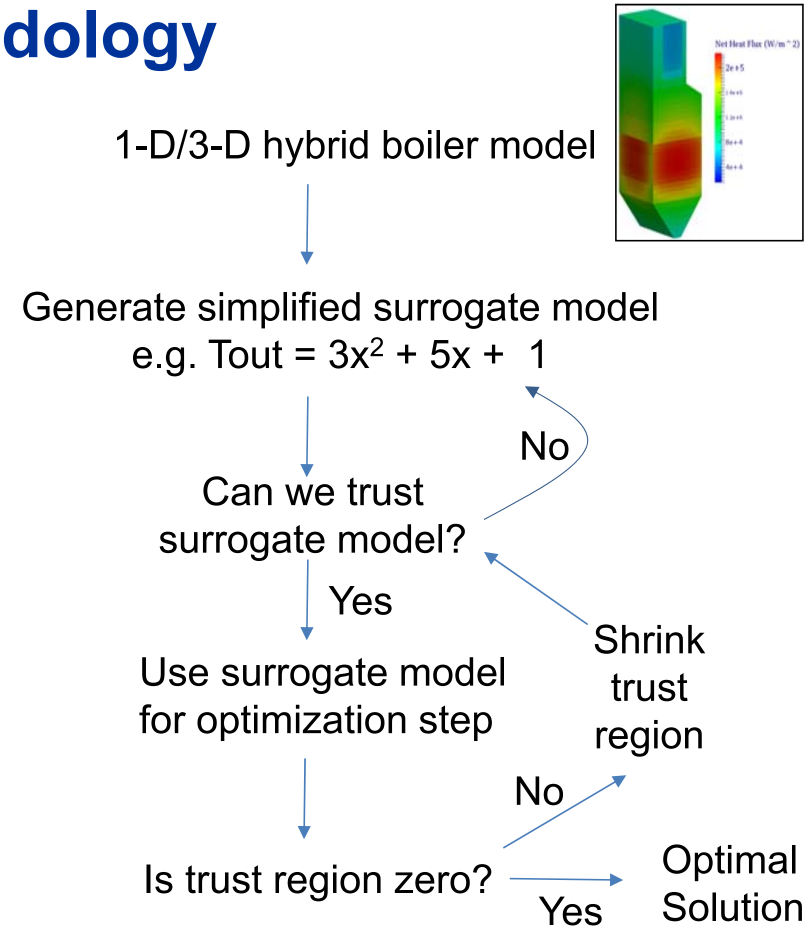
Trust Region Methodology

- Applied for Hybrid Boiler Model

- General idea: Adaptively generate and applies simplified surrogate models throughout the optimization in local domain spaces where it can be trusted.

- Able to prove that the optimal solution to the trust-region problem = optimal solution to original problem



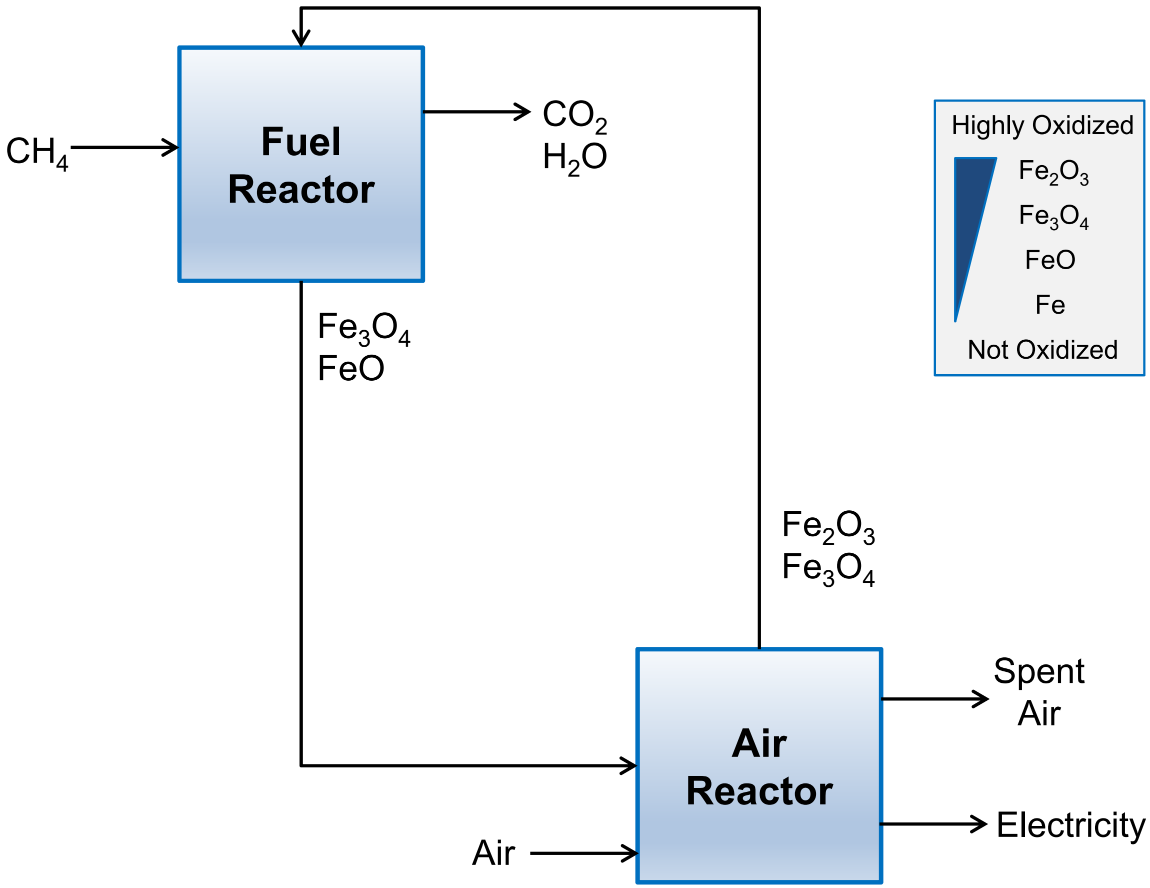
Eason, J. P. and Biegler, L. T. A trust region filter method for glass box/black box optimization. *AIChE J.*, **2016**, 62, 3124–3136.

Oxycombustion Optimization Results

	Air-fired	Oxy-fired
Flue gas temperature (K)	1600	1600
Steam exit temperature (K)	835	835
Steam exit pressure (bar)	223	223
Fuel rate, HHV (MW)	1325.5	1325.5
ASU + CPU Power (MW)	N/A	114.3
Net Power (MWe)	515.5	437.4
Efficiency	38.9%	33.0%

5.9% penalty for oxy-fired configuration

Conceptual Design of Chemical Looping Systems



Equation Oriented Process Optimization

Conceptual Design to Find Optimal Process Configuration

Advanced Process Systems Optimization of Fixed Flowsheets

Results

Optimized Process Configuration and Conditions

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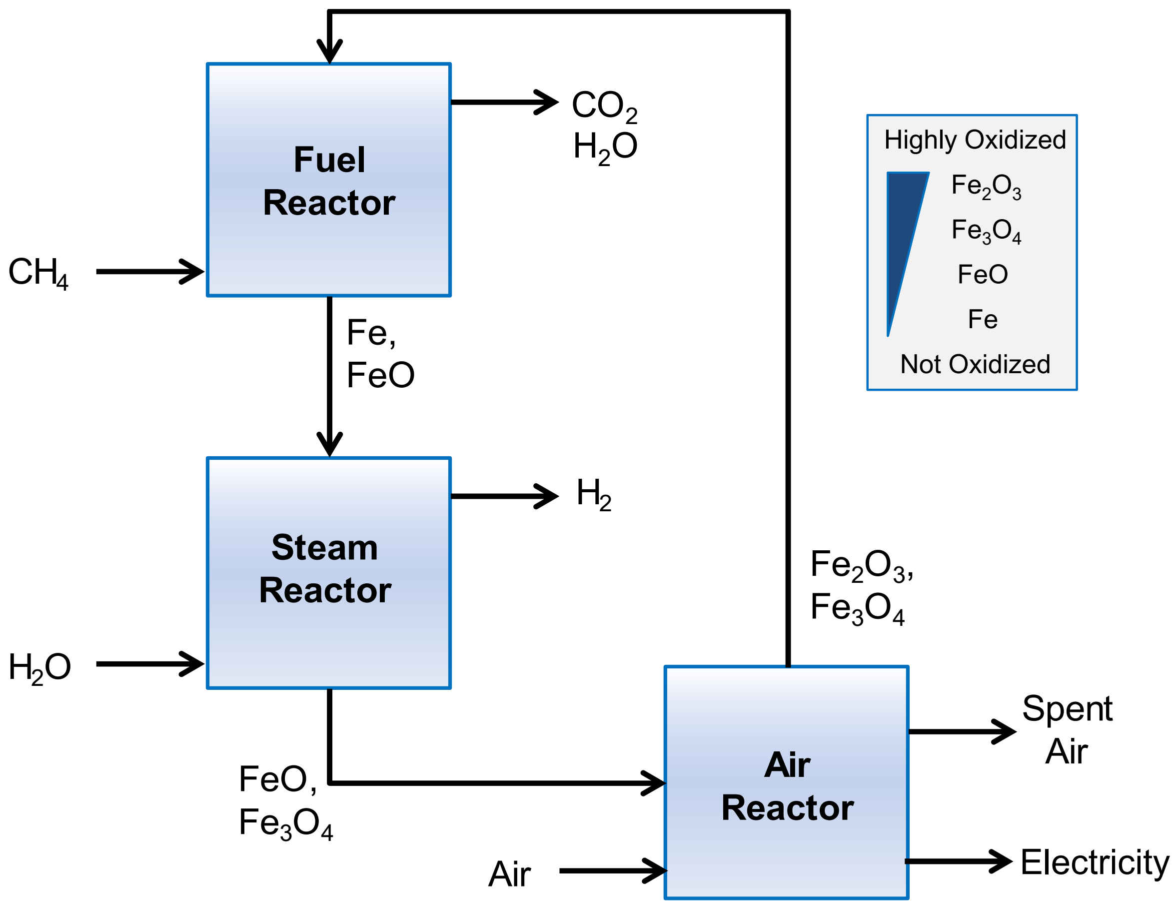
Conceptual Design of Chemical Looping Systems

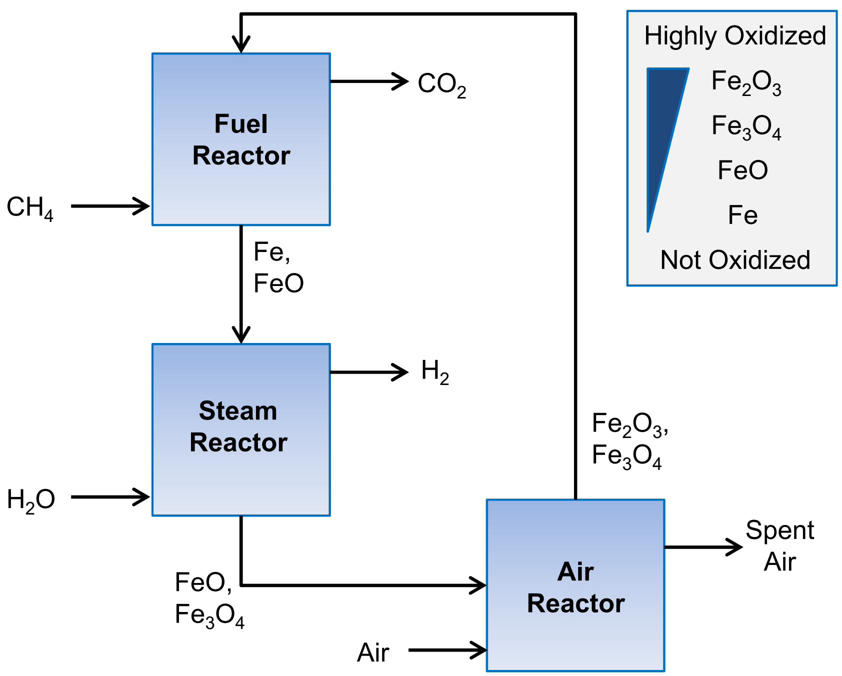


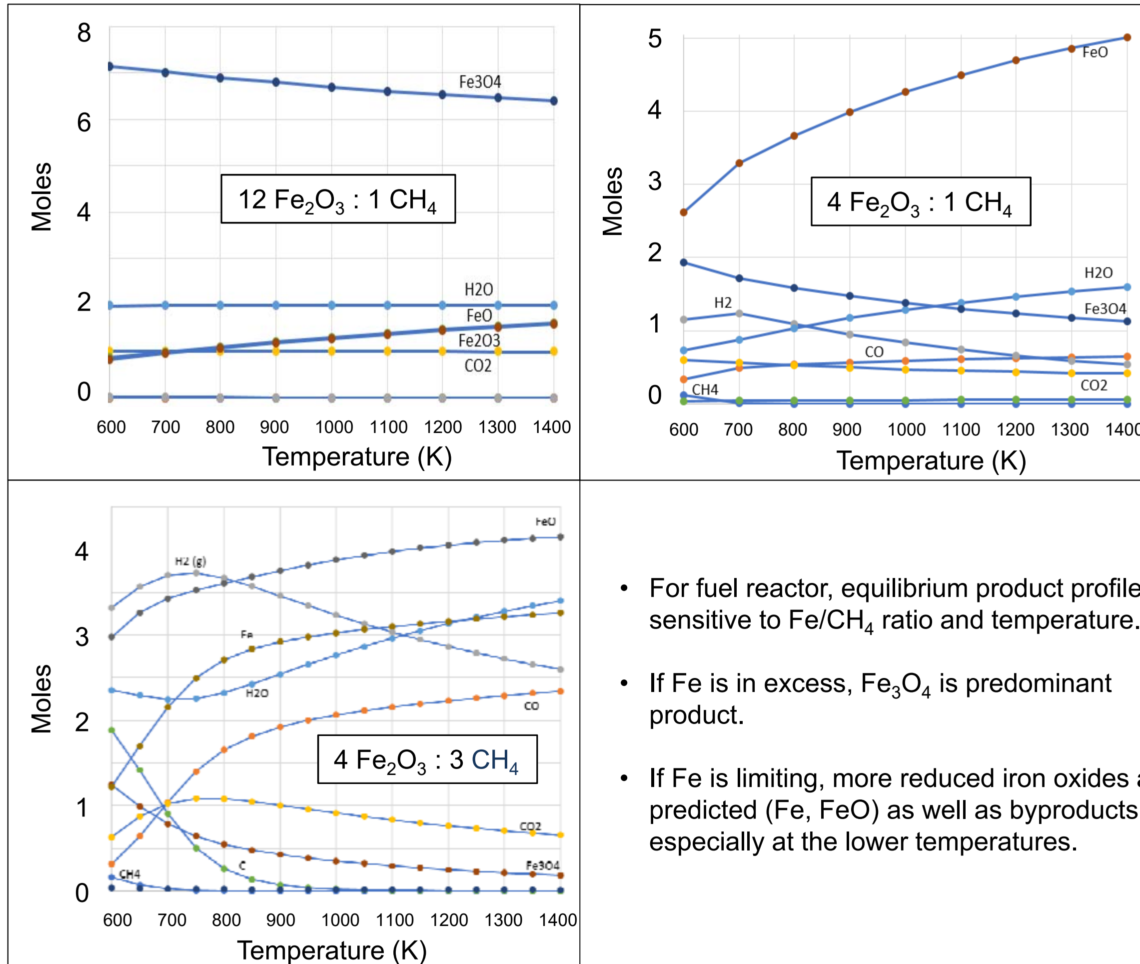
Equation Oriented Process Optimization		Results
Conceptual Design to Find Optimal Process Configuration	➡	Optimized Process Configuration and Conditions
Advanced Process Systems Optimization of Fixed Flowsheets		

Discrete decisions:
- Type, orientation, and number of reactors
- Presence/absence of water-gas shift reactor
- Which products (Power, H_2, Syngas, Heat, CO_2)
- Choice of oxygen carrier

Continuous decisions:
- Operating conditions (temperatures, pressures, flow rates)
- Unit geometries
- Relative amounts of each product

Equilibrium-based Framework for Reactor System





- For fuel reactor, equilibrium product profile is sensitive to Fe/CH_4 ratio and temperature.
- If Fe is in excess, Fe_3O_4 is predominant product.
- If Fe is limiting, more reduced iron oxides are predicted (Fe, FeO) as well as byproducts especially at the lower temperatures.

Next Steps:
- Refine reactor models to include kinetics and hydrodynamics
- Build out chemical looping flowsheet
- Use IDAES Conceptual Design algorithms to optimally chose unit operations and integrate them into complete power system

2016 Major Accomplishments

2. Conceptual Design, Optimization, UQ, and Intensification of Advanced Energy Systems

- Initial **oxycombustion systems model** in Pyomo and compared model predictions with published results
- **Initial chemical looping systems model** in Pyomo and compare model predictions with published results
- Initial optimization framework to determine **size and shape of active metal sites in oxygen carriers**
  - Partnership with NETL's materials development team providing atomistic simulations and experimental results
- **Modeling standards** that can be re-used, linked together, and linked with properties models
- **Framework to automatically generate equation of state property models** from PVT data
- Comprehensive **steady state and dynamic BFB models** for system optimization
- Validated a fully **rate-based solvent system model** in Pyomo with the CCSI Gold Standard MEA model

3. Software Architecture, Algorithms, and Distributed Computing

- Enabled **support of units** within Pyomo
- **Parallel algorithms on the GPU for dense matrices**, and demonstrate them on least squares and parameter estimation problems
- Determined the potential to enable Pyomo to effectively **utilize advanced computing architectures**: NERSC

General

- IDAES was identified as the foundation for an NETL Strategic Initiative
- 10 journal articles and 1 book chapter have been published
- 13 technical presentations were given at national/international scientific conferences

Highlights from Exploratory IDAES Stakeholder Meeting

March 13, 2017
Carnegie Mellon University

- Highly supportive of IDAES
  - Converging on one software tool will solve a multitude of problems
  - Will enable them to becoming more agile in incorporating new capabilities (e.g., latest solvers, cutting-edge academic codes)
  - Will enable extensive customization due to Equation-Oriented optimization approach
  - Will enable quantitative understanding of uncertainty (and risk)
  - Will produce broadly applicable tools that can impact many industries

"I'm glad the government is funding this"

- Early advice
  - Emphasize usability!!!
  - Build it step by step to gather early adopters

Summary

- IDAES is a new computational platform that enables innovation and large, multi-scale system optimization.
- IDAES addresses a number of the challenges associated with the design and scale-up of advanced energy systems.
- The IDAES team is ramping up interactions with technology developers and stakeholders to apply the tools.

Acknowledgements

2. Conceptual Design, Optimization, UQ, and Intensification of Advanced Energy Systems

2.1. Advanced Optimization Strategies for Bubbling Fluidized Bed Processes in Pyomo (2016)

Larry Biegler, Mingzhao Yu, David Molina Thierry

2.2 Advanced Oxycombustion Systems Optimization

Larry Biegler, John Eason, Jinliang Ma, Tony Burgard, Dehao Zhu

2.3 Chemical Looping Systems Optimization

Andrew Lee, Larry Biegler, Mingzhao Yu, David Molina Thierry, Chinedu Okoli

2.4 Molecular design of oxygen carriers for chemical looping

Chrysanthos Gounaris, Chris Hanselman

2.5 Tools for Kinetics and Thermophysical Properties

Nick Sahinidis, Zach Wilson, Marissa Engle, John Eslick

2.6 Advanced Solvent System Optimization

John Eslick, Debangsu Bhattacharyya, Paul Akula

2.7 Conceptual Design Tools

Ignacio Grossmann, Qi Chen, John Siirola, Tony Burgard, Jaffer Ghouse

2.8 Optimal Planning of Electric Power Infrastructures

Ignacio Grossmann, Cristiana Lara, Ben Omell, Joel Theis, Omar Guerra

3. Software Architecture, Algorithms, and Distributed Computing

3.1 System Architecture

John Siirola, Dan Gunter

3.2 Optimization Algorithms and Parallel Computing

Nick Sahinidis, Benjamin Sauk, Dan Gunter, John Siirola

3.3 Data Management and Workflow

Deb Agarwal, You-Wei Cheah

Berkeley
Carnegie Mellon
NETL
Sandia
West Virginia

IDAES-related Publications

- ***Journal publications***
- Ma, J.; Eason, J. P.; Dowling, A. W.; Biegler, L. T.; Miller, D. C., Development of a First-Principles Hybrid Boiler Model for Oxy-Combustion Power Generation System. *International Journal of Green House Gas Control*, **2016**, 46, 136-157
- Eason, J. P. and Biegler, L. T. A trust region filter method for glass box/black box optimization. *AIChE J.*, **2016**, 62, 3124–3136.
- Yu, H.; X. Feng; Y. Wang; L. T. Biegler; J. P. Eason, A systematic method to customize an efficient organic Rankine cycle (ORC) to recover waste heat in refineries, *Applied Energy*, 179, pp. 302-315 (2016)
- Yu, H.; J. P. Eason; L. T. Biegler, Simultaneous heat integration and techno-economic optimization of Organic Rankine Cycle (ORC) for multiple waste heat stream recovery, *Energy*, 119, 322-333 (2017)
- Zhu, D.; J. P. Eason; L. T. Biegler, Energy-efficient CO2 liquefaction for oxy-combustion power plant with ASU-CPU integration enhanced by cascaded cryogenic energy utilization and waste heat recovery, submitted for publication, *International Journal of Green House Gas Control*, **2016**
- Hanselman, C. L.; Gounaris, C. E., A Mathematical Optimization Framework for the Design of Nanopatterned Surfaces. *AIChE Journal* **2016**, *62* (9), 3250-3262
- Chen, Q.; Grossmann, I. E., Recent developments and challenges in optimization-based process synthesis. *Annual Review of Chemical and Biomolecular Engineering*. [accepted]
- Wilson, Z.; Sahinidis, N. V., The ALAMO methodology for machine learning. Computers and Chemical Engineering. [submitted]
- Sauk, B.; Ploskas, N.; Sahinidis, N. V., GPU parameter tuning for dense linear least squares problems. *Parallel Computing*. [submitted]
- Barnett, J.; Watson, J.-P.; Woodruff, D.L., BBPH: Using Progressive Hedging Within Branch and Bound to Solve Multi-Stage Stochastic Mixed Integer Programs. *Operations Research Letters*, [accepted].
- ***Book chapters***
- Dowling, A. W., J. P. Eason, J. Ma, D. C. Miller and L. T. Biegler (2016). Equation-Based Design, Integration, and Optimization of Oxycombustion Power Systems. Alternative Energy Sources and Technologies: Process Design and Operation. M. Martín. Cham, Springer International Publishing**:** 119-158.

IDAES-related Conference Presentations

- ***Conference papers/presentations***
- Yu, M.; Biegler, L. T., A Stable and Robust NMPC Strategy with Reduced Models and Nonuniform Grids. Proceedings of the 11th IFAC Symposium on Dynamics and Control of Process Systems, pp.31-36, 2016
- Yu, M.; Biegler, L. T., Economic Nonlinear Model Predictive Control of an Integrated Solid-Sorbent Carbon Capture System," paper 488a, presented at Annual AIChE Meeting, San Francisco, CA, November, 2016
- Eason, J.P. and Biegler, L.T. Large-scale optimization with multi-scale models. Presented at Workshop on Nonlinear Optimization Algorithms and Industrial Applications, Toronto, ON, Canada. 2 June 2016.
- Eason, J.P. and Biegler, L.T. A trust region method for glass box/black box optimization. Presented at The Fifth International Conference on Continuous Optimization (ICCOPT), Tokyo, Japan. 9 August 2016.
- Eason, J.P. and Biegler, L.T., Rigorous Surrogate-Based Optimization Strategies That Integrate Glass Box/Black Box Process Models, paper 514g, presented at Annual AIChE Meeting, San Francisco, CA, November, 2016
- Hanselman, C. L.; Gounaris, C. E., Rational design of nanostructured metallic surfaces via mathematical optimization. In the *AIChE Annual Meeting*, San Francisco, CA, 2016.
- Hanselman, C. L.; Gounaris, C. E., A mixed-integer linear programming approach for the design of nanostructured catalysts. In the *AIChE Annual Meeting*, San Francisco, CA, 2016.
- Chen, Q.; Grossmann, I.E., Towards a computational platform for general flowsheet synthesis. In *AIChE Annual Meeting*, San Francisco, CA, 2016.
- Lara, C.L.; Grossmann, I.E., MILP Formulation for Optimal Planning of Electric Power Infrastructures. In *AIChE Annual Meeting*, San Francisco, CA, 2016.
- Siirola, J.D.; Hart, W.E; Laird, C.D.; Nicholson, B.L.; Watson, J.-P.; Woodruff, D.L., Recent developments in Pyomo. In *5th International Conference on Continuous Optimization*, Tokyo, Japan, 2016.
- Siirola, J.D.; Hart, W.E; Laird, C.D.; Nicholson, B.L.; Watson, J.-P.; Woodruff, D.L., Recent developments in Pyomo. In *2016 AIChE Annual Meeting*, San Francisco, California, 2016.
- Nicholson, B.L. and Siirola, J.D. A Framework for Modeling and Optimizing Dynamic Systems Under Uncertainty. *Accepted for presentation at FOCAPO/CPC 2017.* Tucson, Arizona, 2017.
- Siirola, J.D.; Watson, J.-P.; Woodruff, D.L., Accelerating and automatic tuning for Progressive Hedging, In *XIV International Conference on Stochastic Programming.* Buzios, Brazil, 2016

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