IDAES

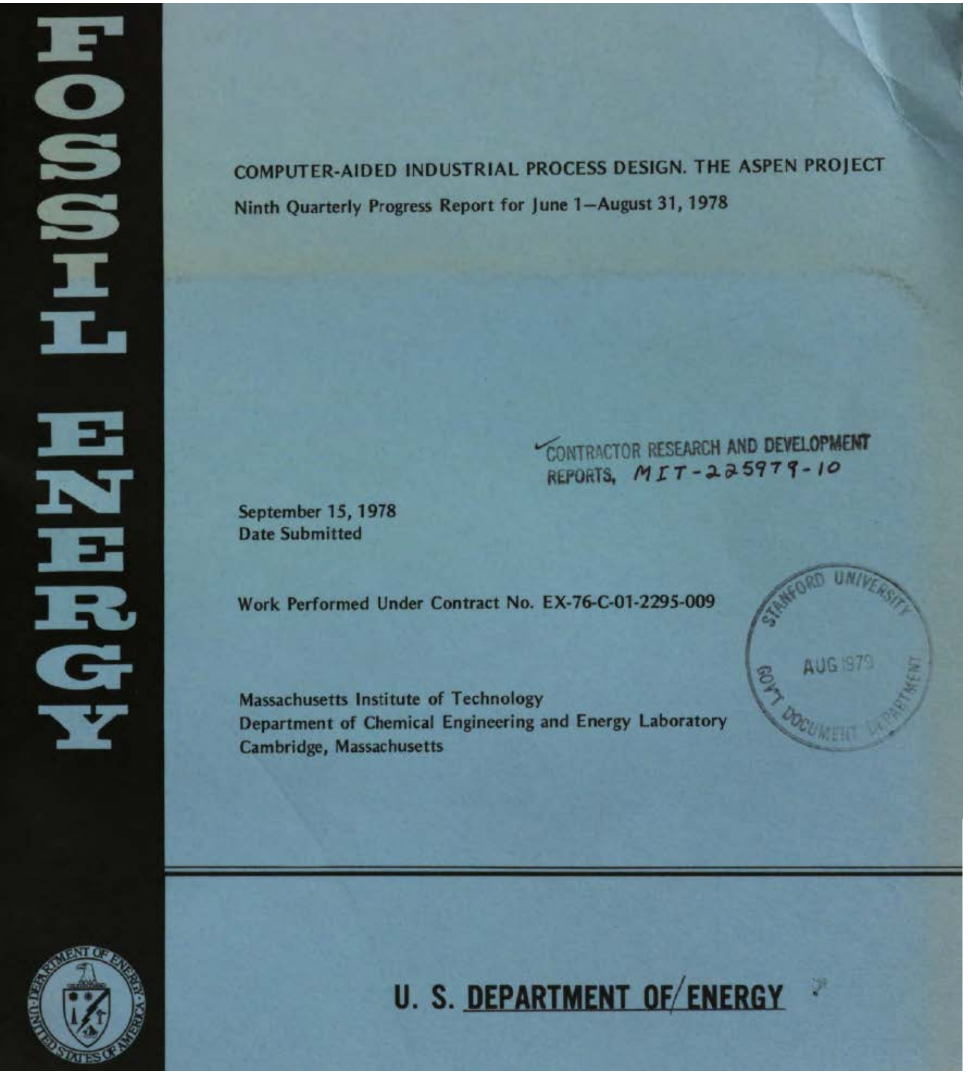
Institute for the Design of Advanced Energy Systems

David C. Miller

April 2019

NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Sandia National Laboratories · Carnegie Mellon · West Virginia University · U.S. DEPARTMENT OF ENERGY

DOE/FE History of Innovation for PSE: Original Aspen


FOSSIL ENERGY

COMPUTER-AIDED INDUSTRIAL PROCESS DESIGN. THE ASPEN PROJECT

Ninth Quarterly Progress Report for June 1—August 31, 1978

CONTRACTOR RESEARCH AND DEVELOPMENT REPORTS, MIT-225979-10

September 15, 1978
Date Submitted

Work Performed Under Contract No. EX-76-C-01-2295-009

Massachusetts Institute of Technology
Department of Chemical Engineering and Energy Laboratory
Cambridge, Massachusetts

U. S. DEPARTMENT OF ENERGY

COMPUTER-AIDED INDUSTRIAL PROCESS DESIGN

The ASPEN Project

First Annual Report
for the period
June 1, 1976 to May 30, 1977

PREPARED FOR THE UNITED STATES
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
FOSSIL ENERGY PROGRAM

Under Contract No. E(49-18)-2295 Task No. 9

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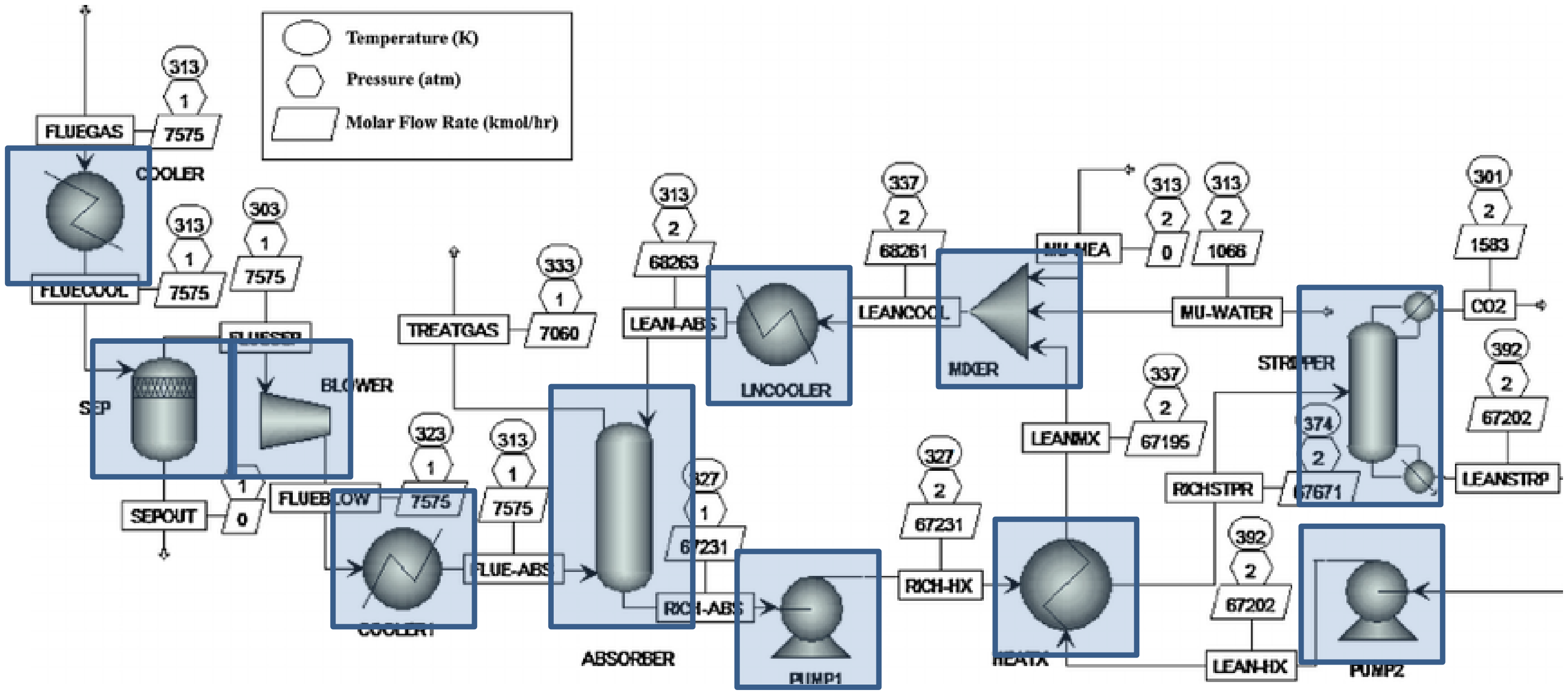
Sequential Modular Process Flowsheet Simulation



Kundu, Prodip & Chakma, Amit & Feng, Xianshe. (2014). Effectiveness of membranes and hybrid membrane processes in comparison with absorption using amines for post-combustion CO2 capture. International Journal of Greenhouse Gas Control. 28. 248–256.

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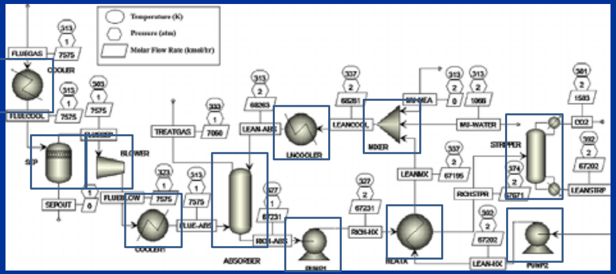
Process Optimization: Transition to EO (algebraic) models

Optimization over degrees of freedom only

$$\min_{u} \quad f(u)$$
$$u^L \le u \le u^U$$

u ↓ ↑ f

Simulator



Black-box optimization (DFO)
~ 100-1000 simulations

[Adapted from Biegler, 2017]

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Process Optimization: Transition to EO (algebraic) models

Optimization over degrees of freedom only

$$\min_{u} \; f(u)$$
$$u^L \leq u \leq u^U$$

↓ u ↑ f

Simulator

$$h(x,u)=0$$

Black-box optimization (DFO)
~ 100-1000 simulations

Glass-box optimization
~ 1-5 STE

Optimization with embedded algebraic model as constraints

$$\min_{x,u} \; f(x,u)$$
$$h(x,u)=0$$
$$x^L \leq x \leq x^U$$
$$u^L \leq u \leq u^U$$

[Adapted from Biegler, 2017]

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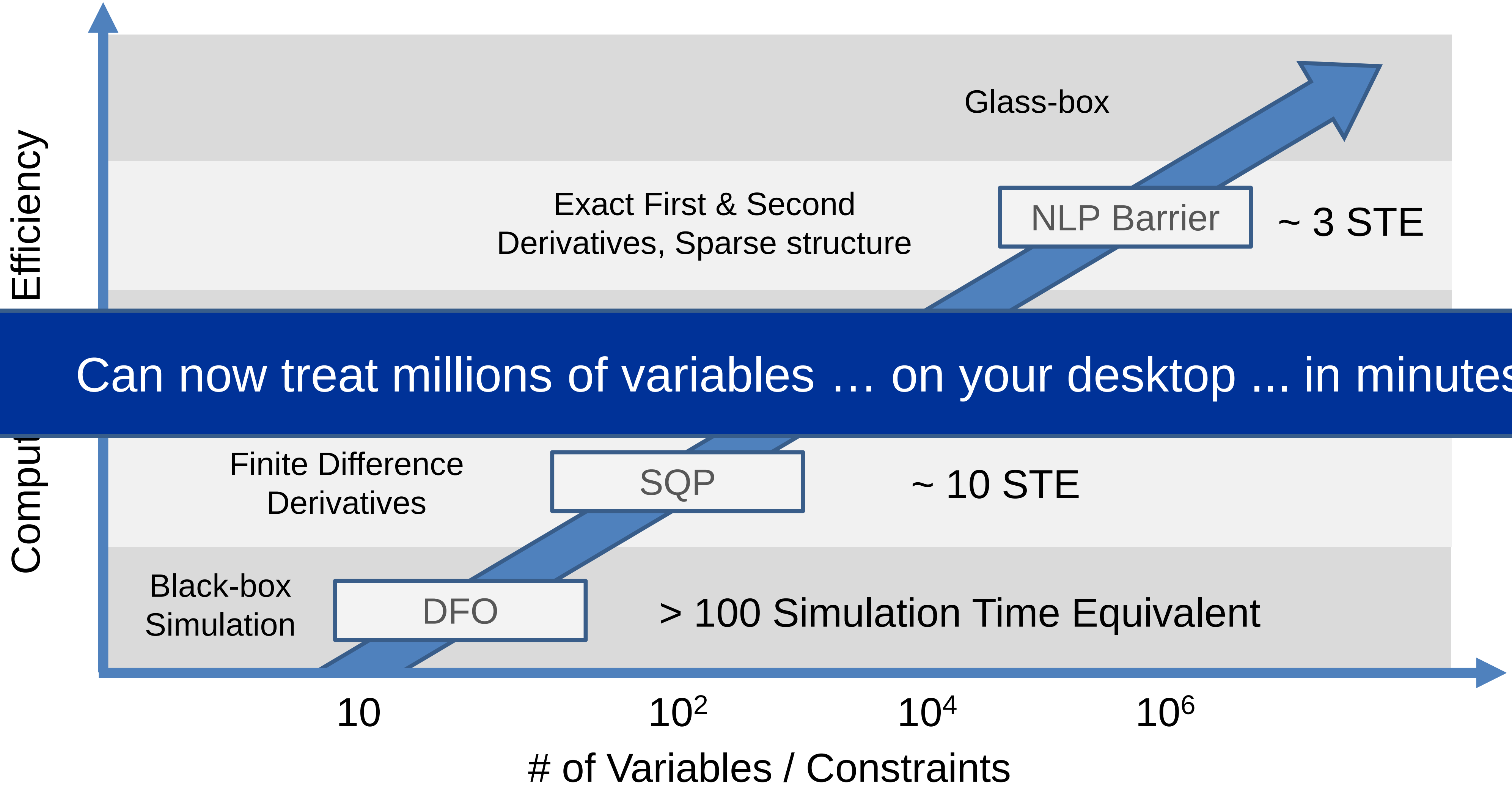
Process Optimization Environments and NLP Solvers



Can now treat millions of variables … on your desktop ... in minutes

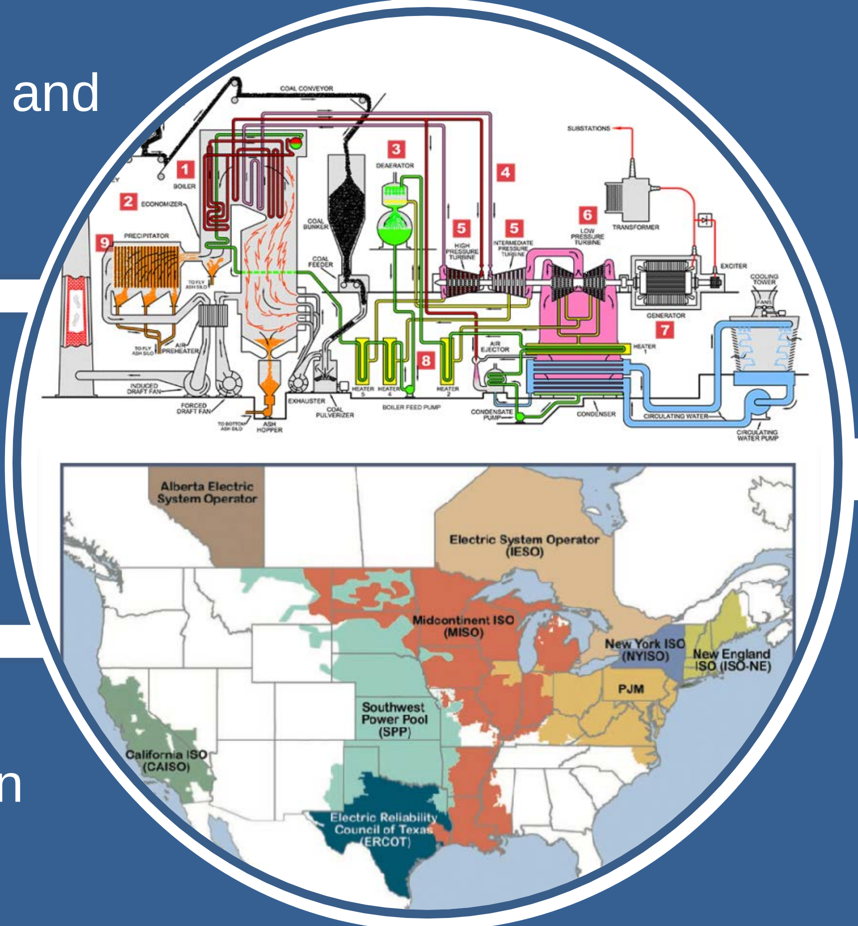
[Adapted from Biegler, 2017]

IDAES: Built on Fundamental Advances in Algorithms & Hardware

Transition to glass-box modeling and analysis (algebraic, glass-box)

Advances in continuous nonlinear optimization (dynamics, uncertainty)

Advances in discrete optimization (algorithms and formulation)



Open-source, extensible algebraic modeling platforms

Emerging computational architectures and high-performance computing

Challenges that IDAES is Addressing

Support for the existing fleet

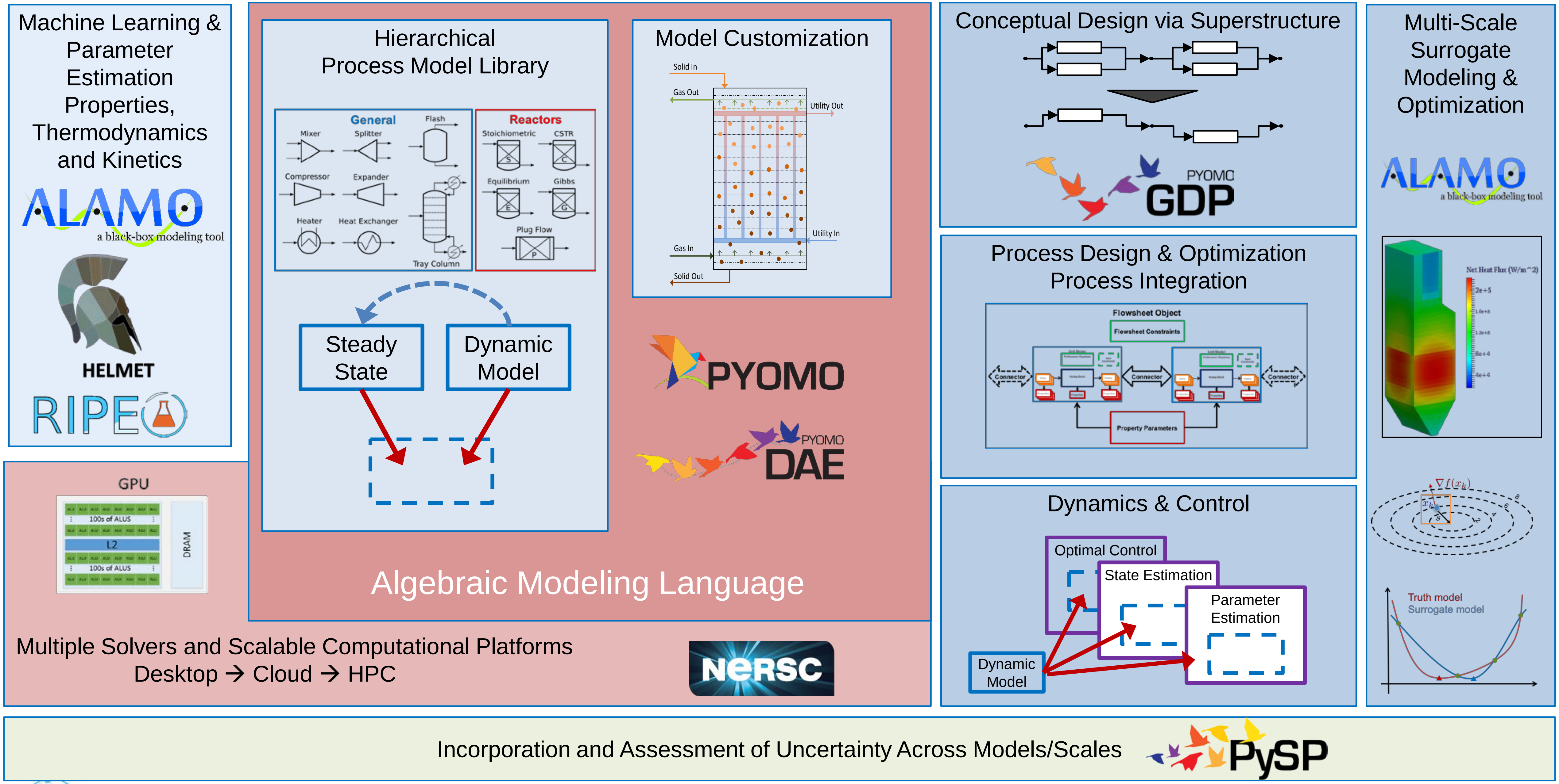
- Optimization of operations to improve efficiency, flexibility
- Evaluation improvement options
- Evaluate in the context of grid

Support development of future advanced energy systems

- Evaluate design options: modular, process intensification, new technology
- Flexible, dynamic designs
- Support development and scale up
- Optimize new materials
- Confirm viability of new ideas in market context, set cost/performance targets

Support development and operation of new processes

- Carbon utilization
- Other process technology



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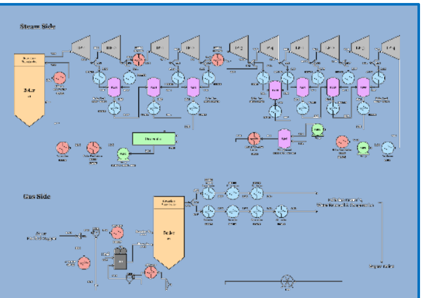
IDAES Approach to Modeling and Optimization

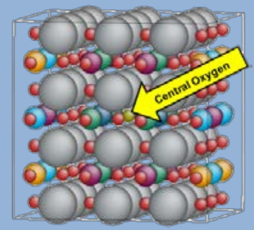
Data	Submodels	Problem Formulation
Experimental Data	Thermo-Physical Properties Reaction Kinetics and Equilibrium Heat and Mass Transfer	Unit Models Flowsheets
Computational Chemistry Experimental Data	Molecular Descriptors	Mathematical Model Motifs and Structure
Grid Data from ISO Generator Cost/Performance Data Transmission Data Load/Demand Curves	Representative Dispatch Days Supply/Demand Models	Multi-Scale Infrastructure Planning Model

Data Management Framework

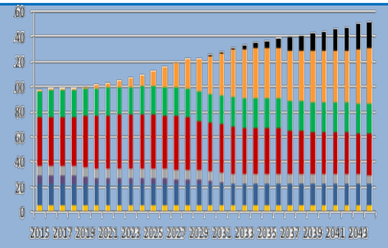
Transformations
Initialization
Solvers



Process Systems

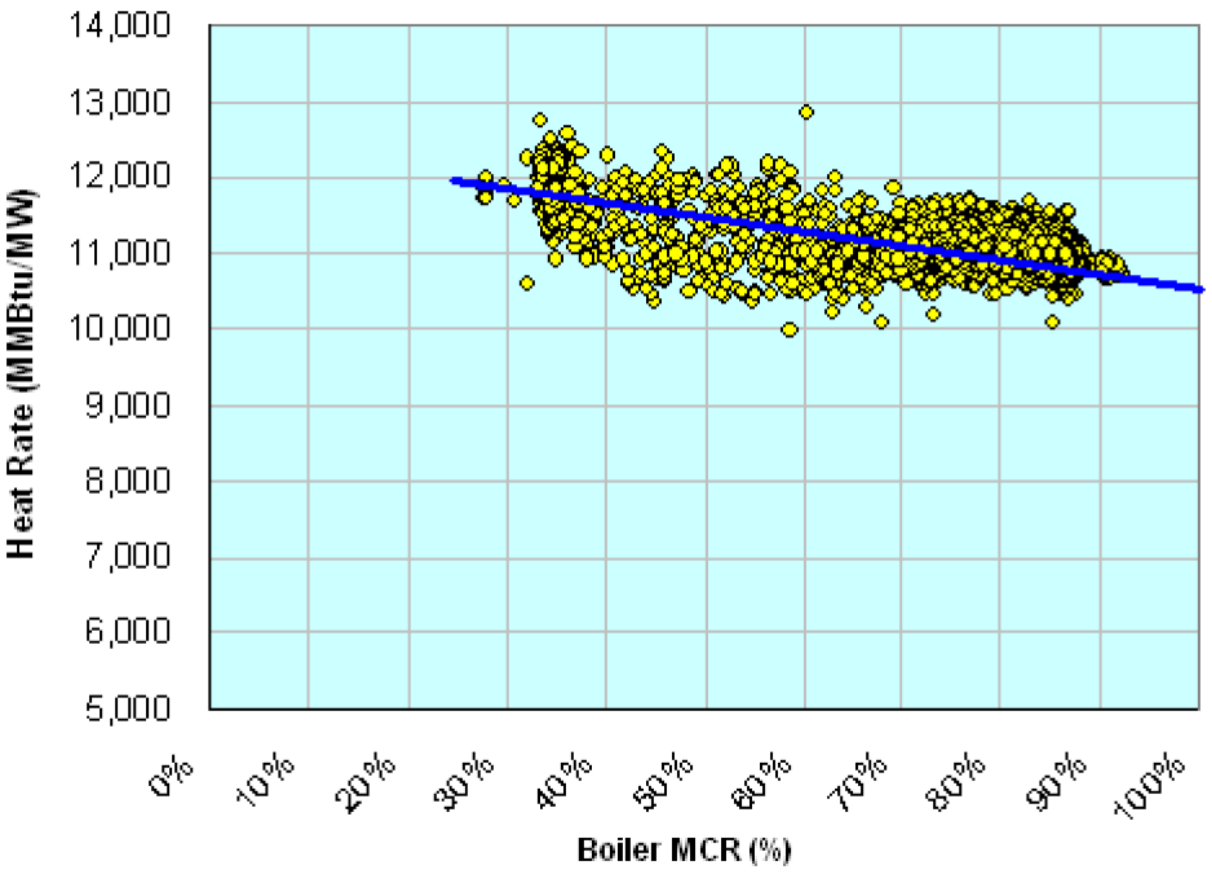


Materials Optimization



Energy Market Model

Support for the Existing Fleet



* Figure source: Power Generation Energy Efficiency Opportunity Identification Report, ABB, 2010

- Data reconciliation
- Parameter estimation
- Steady-state optimization
- Dynamic optimization

- Deploy IDAES software Power Station mid-2020
- General steady-state and dynamic model libraries released 2019, 2020

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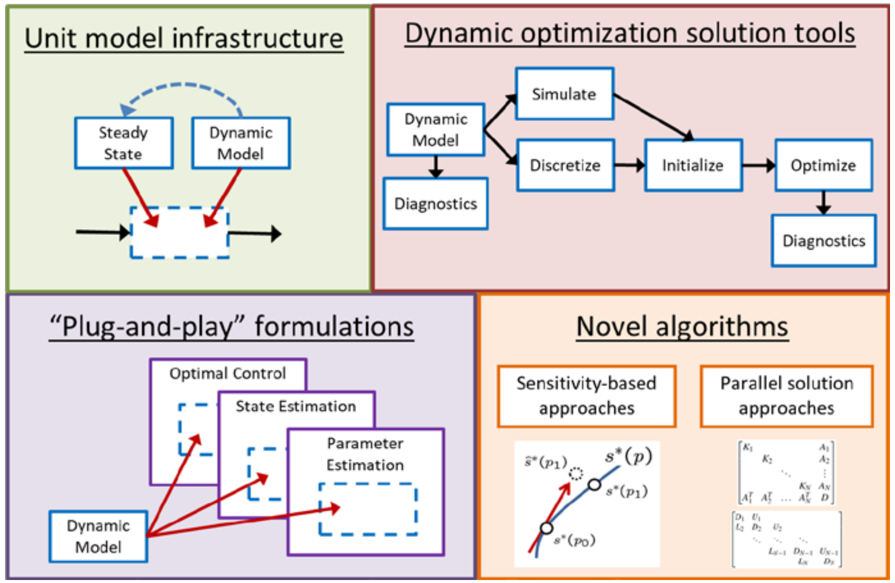
Advanced Dynamic Optimization Capabilities

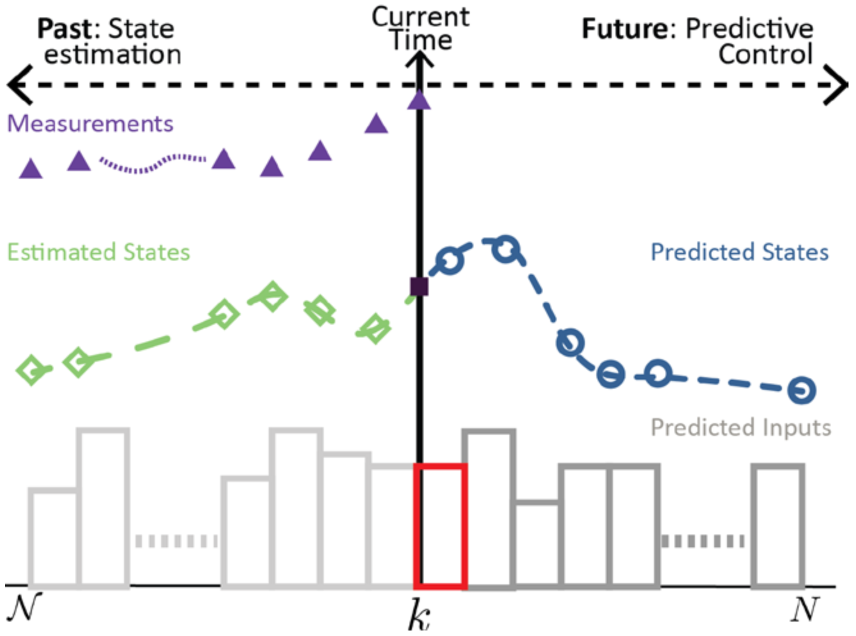


- **Dynamic model development and validation**
  - Convergence testing
  - Model identification and parameter estimation
- **Time-scale based model reduction**
  - Remove fast states
  - Create ‘fast’ models that accuracy
- **Nonlinear state estimation and control**
  - Required for optimizing start-up/shutdown, ramping
  - Simplify and streamline the implementation process and enable code re-use by separating the dynamic model from the specific problem formulation
- **Decomposition-based, parallel solution algorithms**
  - Exploit structure imposed by time/spatial discretization to solve larger-scale (e.g. full power plant) problems

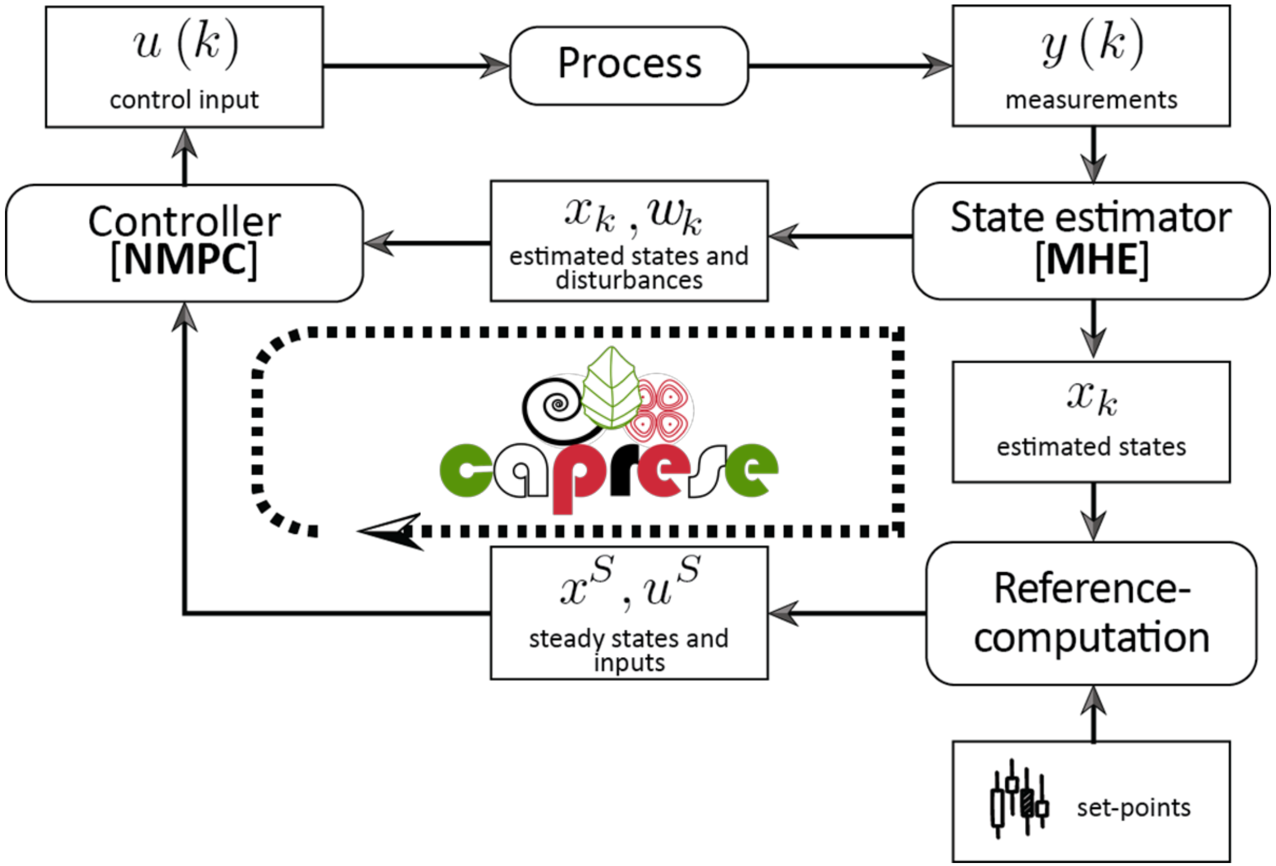
Dynamics and Advanced Process Control in IDEAS
Bethany Nicholson, David Thierry, Robert Parker,
Jose Rodriguez, Carl Laird, Lorenz Biegler

Nonlinear State Estimation and Control

MHE coupled with NMPC



Software Framework



Exploring New Opportunities for Plant Participation

- **Power plants do not operate in a vacuum**
  - Participation (revenue) determined by interaction with the grid energy and service markets
  - Quantifying potential benefits (increased revenues) for operating coal plants in more dynamic regimes induced by changing grid conditions

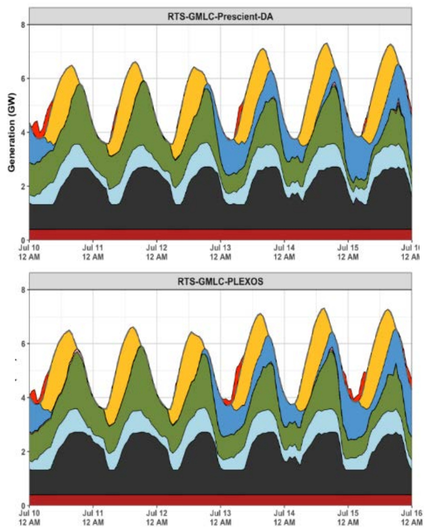
- **Key technology: Prescient**
  - DOE-developed (SNL/NREL) Production Cost Modeling tool
  - Simulates the operation of a grid at an hourly resolution for extended periods
  - Verified against commercial PCM tools (PLEXOS, PSO)

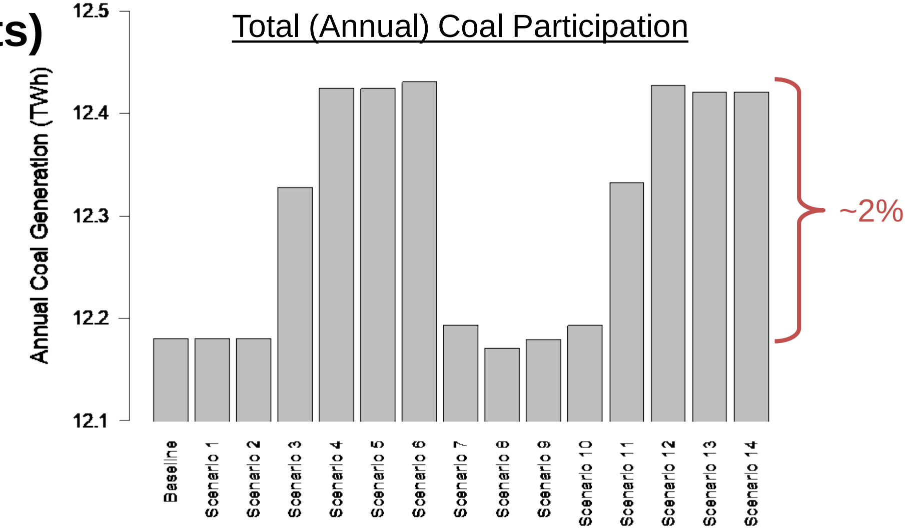
- **Initial studies using RTS-GMLC test system (19% coal – 16 plants)**
  - Vary plant ramp rates, minimum up/down times
  - Total coal participation could be changed by ~2%
    - Although individual plants could change by up to 10%
  - Ramp limits did not impact operations at the hourly scale

- **Current activities: increase simulation fidelity**
  - Adding short-term (5-minute) markets to Prescient
  - Adding ancillary service markets to Prescient

Prescient

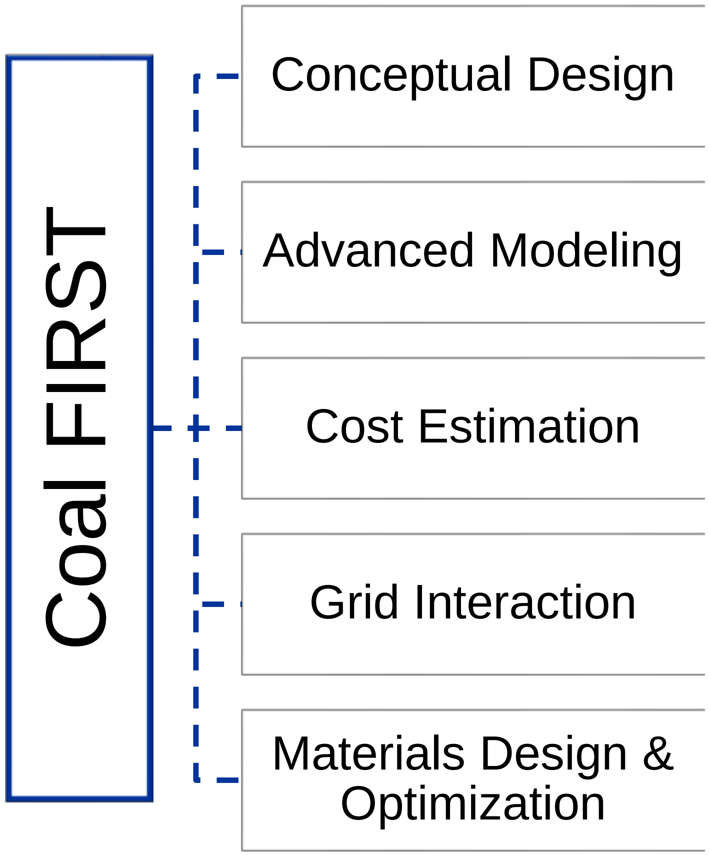
PLEXOS





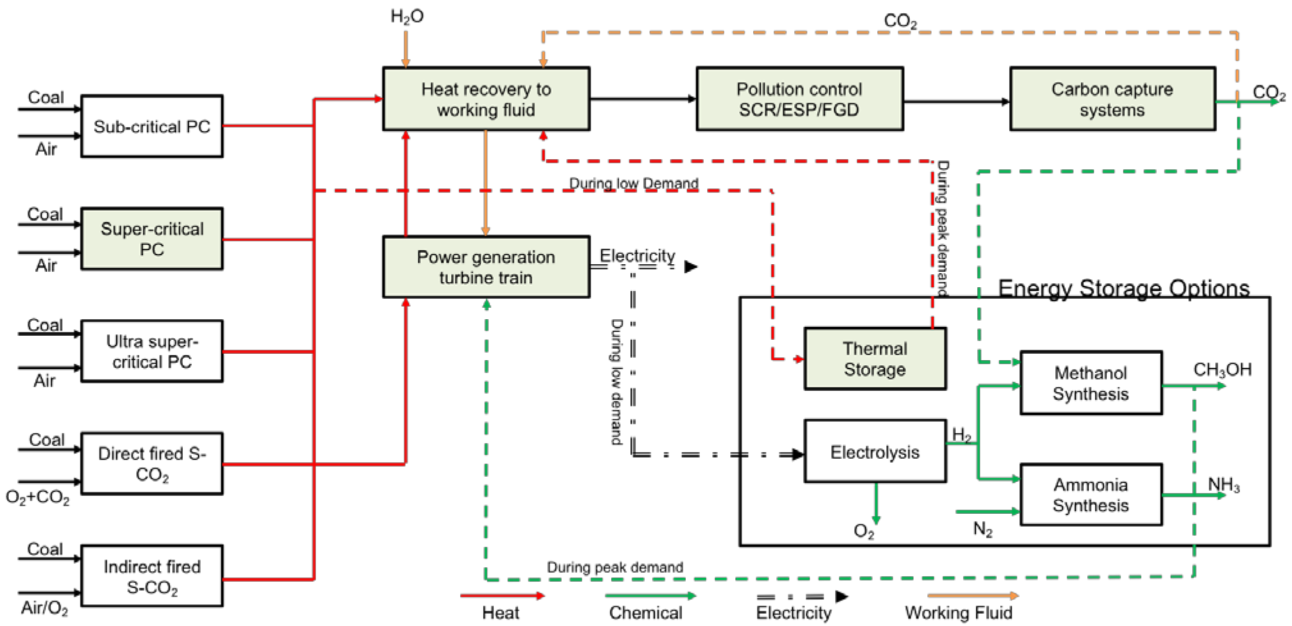
Designing Coal FIRST Power Plants

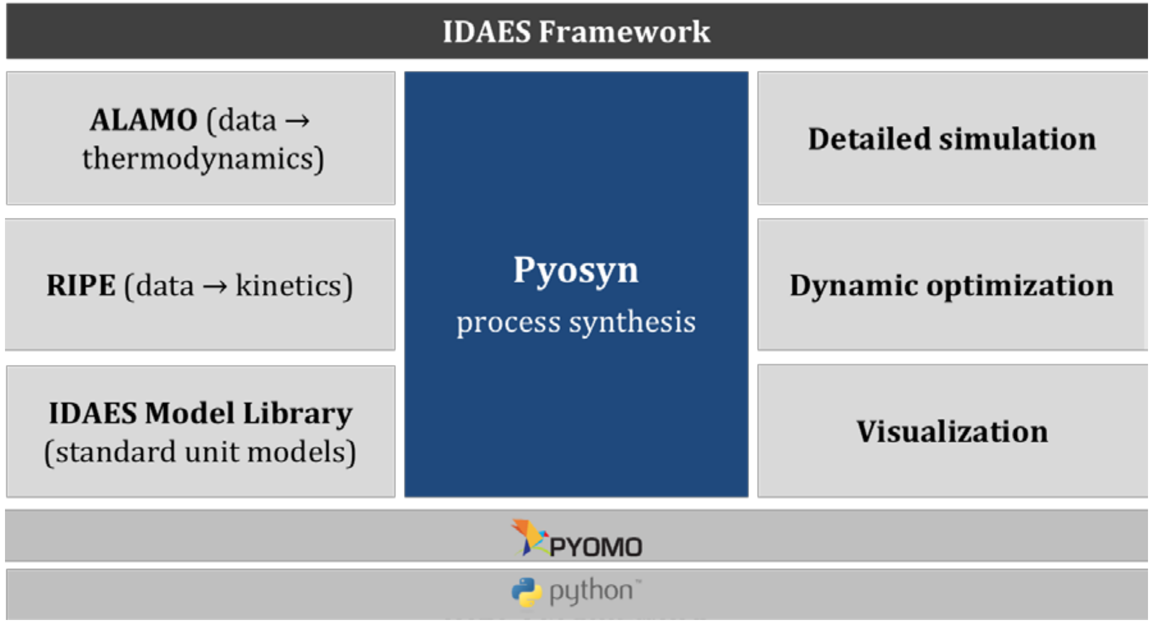
Flexible, Innovative, Resilient, Small and Transformational



Conceptual Design of Coal FIRST Power Plants

- **Large space of flowsheet design options (upstream technologies, firing, storage, emissions, etc.)**
- **Need for flexible, resilient operations to respond to both national and market needs of the electrical grid**





- Current focus: (1) Integration of Pyosyn with the IDAES framework, (2) Conceptual design models for integrated energy storage, and (3) Algorithm development to support large-scale conceptual design.
- Long-term goals: ◆ Rich library of conceptual design models ◆ Superstructure optimization of Coal FIRST powerplant (including traditional and novel upstream options) ◆ Extension of conceptual design tools for uncertainty and multi-objective problems ◆ Tools and analysis for modular designs

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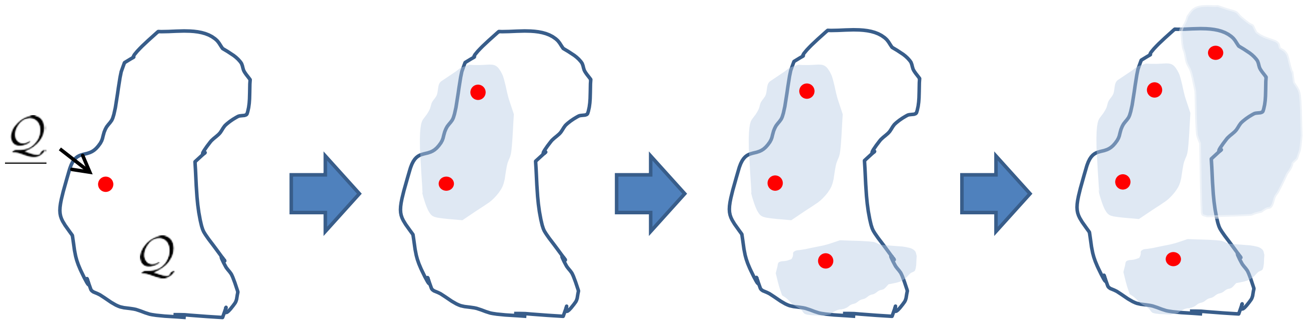
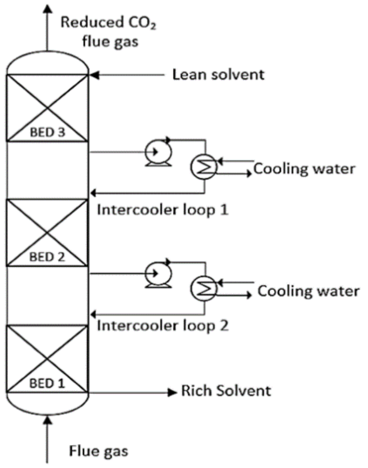
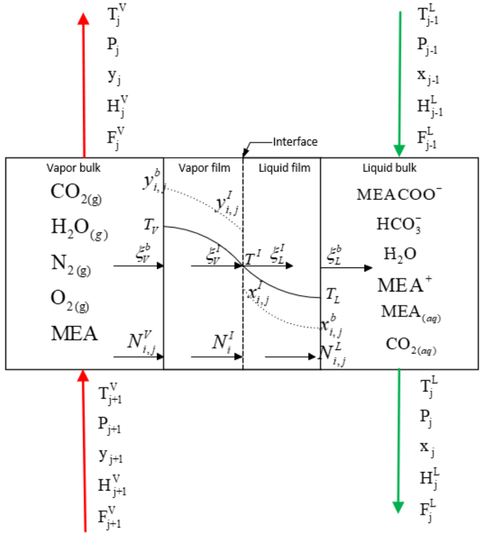
Incorporating Uncertainty into Process Design

- **Developing general algorithms for Nonlinear Robust Optimization**
  - Enable optimal design of equipment, even in the presence of data uncertainty (e.g., from physical property models or from predicted performance of new materials
  - Initial approach: Robust Cutting Sets
    - Case study: design of an absorber column







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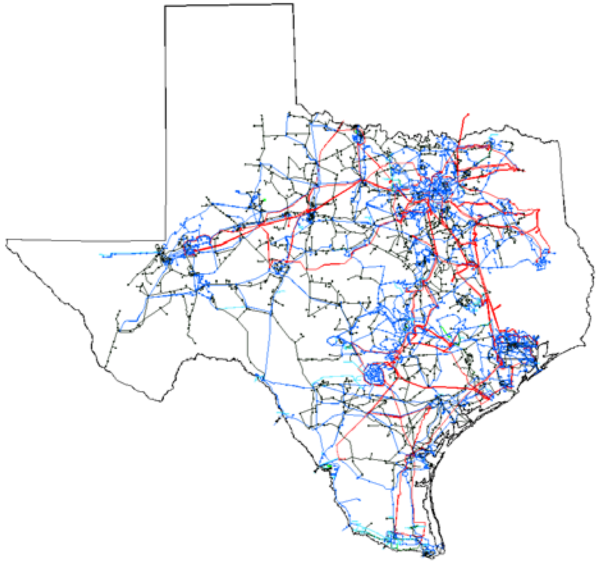
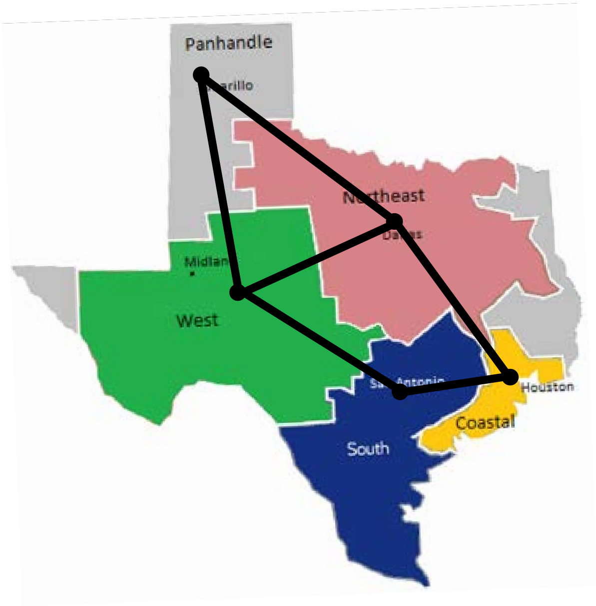
Coal FIRST Expansion Planning

- **Will new technology be adopted?**
  - Plants will be built if they are *profitable.*
  - Profitability implies that they help the grid provide reliable power at the *lowest cost to consumers*

- **Multi-stage stochastic programming (MSSP) algorithms**
  - Expansion planning models
    - Long-term (20-30+ year) grid planning models
    - Significant uncertainties over those periods
- **Implementing bidding curve rolling horizon framework**
    - Eventual goal to integrate with Prescient (dispatch model)





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Partnership and Impact

Stakeholder Advisory Board (May 16-17 @ Bethesda, MD)

- Keep informed of developments, progress
- Provide input on key challenges

Collaborate with IDAES to apply the tools

- Cooperative Research & Development Agreement (CRADA)
  - Protects IP, enables information sharing
- Existing Coal-Fired Power Plant
- Chemical Looping
- Opportunities to apply to problems in your domain

Join the IDAES development community (Open Source Release Available)

- Access to IDAES Computational Framework
- Opportunity to expand capabilities of the tools

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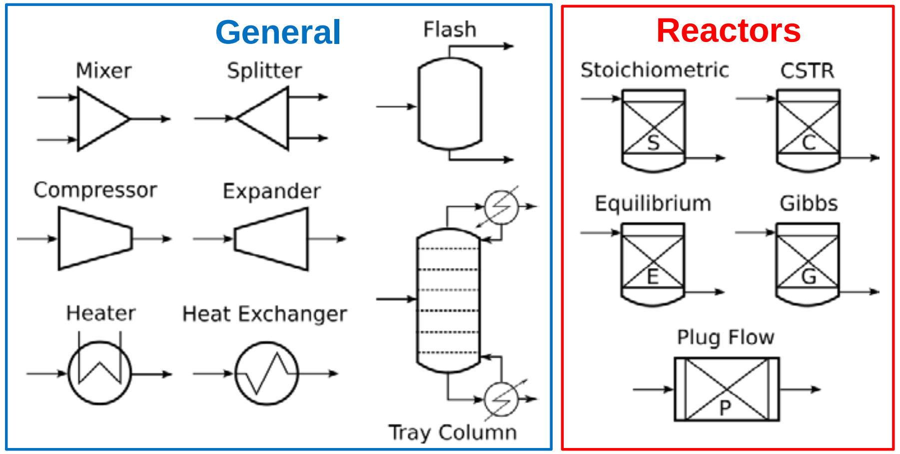
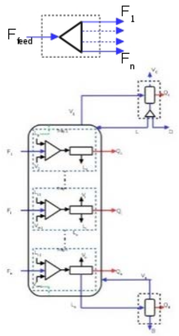
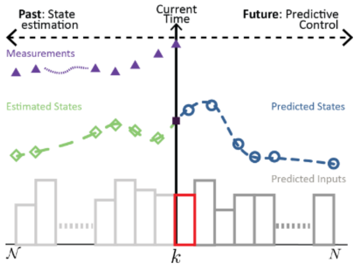
IDAES PSE Framework Released via Github

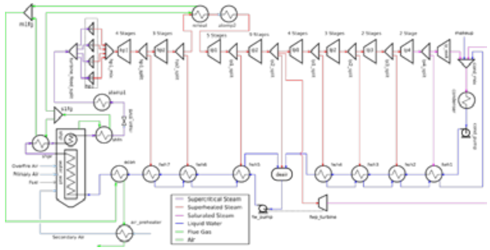
- IDAES received DOE permission to assert copyright and release the IDAES Framework

- Permissive licensing (revised BSD)
  - No restrictions on commercial use
  - No requirement that you share derivative works / modifications (*not* "copy-left")
  - We only ask for acknowledgement
- Initial capabilities:
  - Model library
  - Conceptual design
  - Dynamic modeling
  - Example power plant flowsheet









Documentation and Learning Materials

- Documentation now hosted on “www.readthedocs.org”
- Initial tutorials
  - Jupyter notebook examples (2) in an interactive environment
    - https://idaes.github.io/idaes-pse/examples/Tutorial_1_Basic_Flowsheets.html
  - New tutorials will be added
- Advanced tutorials (in development)
  - Building custom unit models and property packages
  - Using Pyomo tools for model analysis
- Exploring video tutorials (especially focused on “getting started” in IDAES)
- Investigating JupyterHub to host tutorials (no installation required)
- Exploring other distribution options (docker containers)
- Planned workshops:
  - Stakeholder meeting demo/workshop (May 16-17)
  - FOCAPD meeting hands-on workshop (July 14-18)
    - Targeted to a broader PSE audience

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We graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy, through the Crosscutting Research Program and the Advanced Combustion Systems Program.

The IDAES Technical Team:

- **National Energy Technology Laboratory**: David Miller, Tony Burgard, John Eslick, Andrew Lee, Miguel Zamarripa, Jinliang Ma, Dale Keairns, Jaffer Ghouse, Emmanuel Ogbe, Gary Kocis, Ben Omell, Chinedu Okoli, Richard Newby, Grigorios Panagakos, Maojian Wang
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- **Lawrence Berkeley National Laboratory**: Deb Agarwal, Dan Gunter, Keith Beattie, John Shinn, Hamdy Elgammal, Joshua Boverhof, Karen Whitenack
- **Carnegie Mellon University**: Larry Biegler, Nick Sahinidis, Chrysanthos Gounaris, Ignacio Grossmann, Owais Sarwar, Natalie Isenberg, Chris Hanselman, Marissa Engle, Qi Chen, Cristiana Lara, Robert Parker, Ben Sauk, Vibhav Dabadghao, Can Li, David Molina Thierry
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For more information visit us at: **https://idaes.org/**

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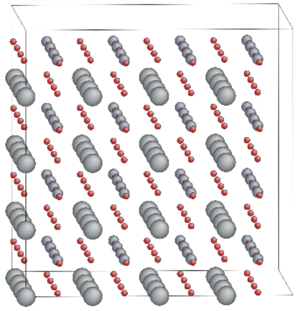
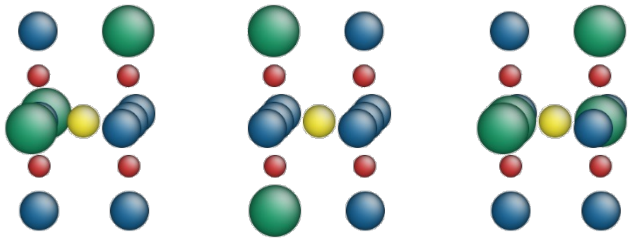
Materials Design & Optimization

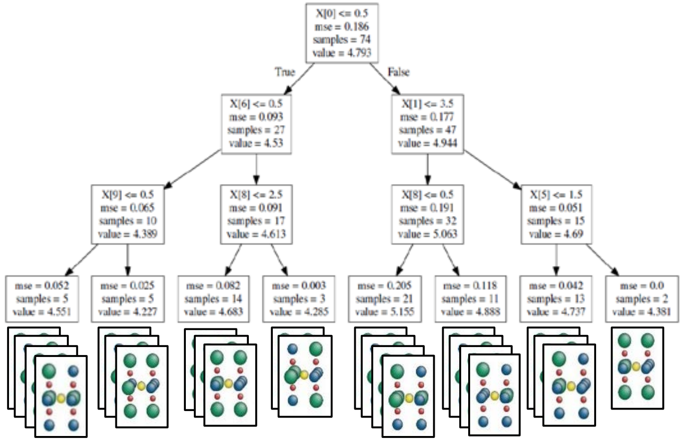


Problem Definition



-1.51 eV   -1.47 eV   -1.47 eV   …

Structure Evaluation



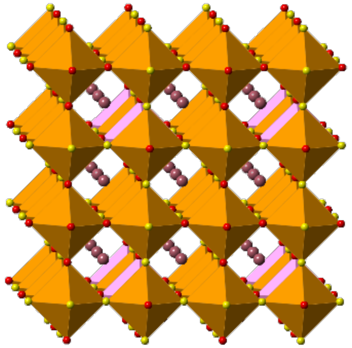
Structure-Function Relationship Identification

Iterative Model Refinement

Mathematical Optimization

$$\min_{s \in S} \quad F(s)$$
$$\text{s.t.} \quad G(s) \leq 0$$

Candidate Optimal Structures



- **Ongoing Work:**
  - ➢ Expanding perovskite model (e.g., formation energy, multiple O removal)
  - ➢ Automated tool to cast material optimization problems
  - ➢ Investigating structure-function relationships for High Entropy Alloys (HEAs)

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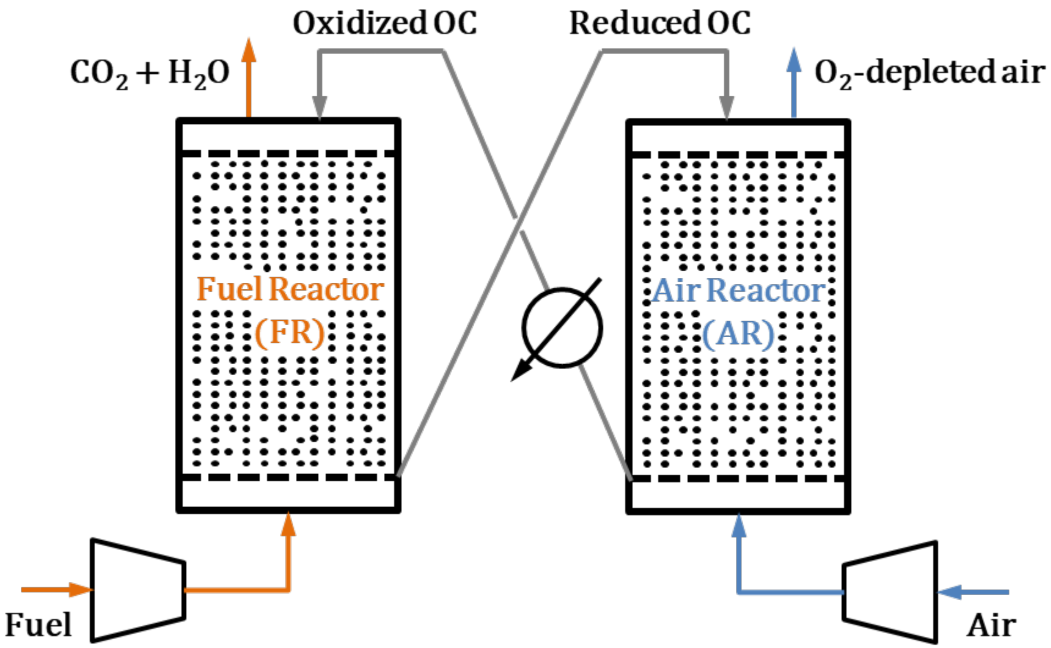
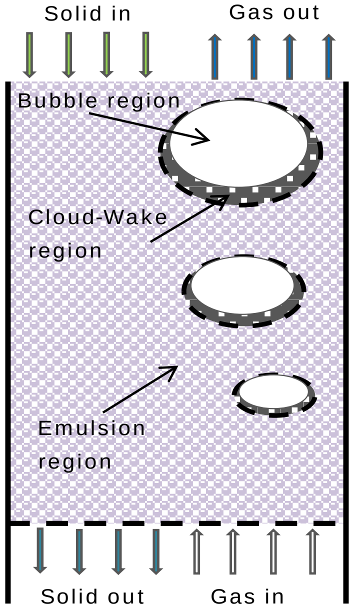
Chemical Looping Combustion



FY-19 Scope (OSU Collaboration)

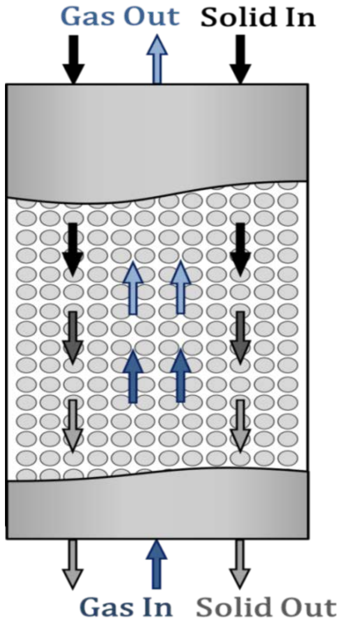
- Kinetic models for OSU oxygen carrier
- Reactors capable of handling solid fuels
- Dynamic models for startup/shutdown, control
- Model validation



Bubbling Fluidized Bed

Model Features

- Equation oriented PDAEs
- Automated sequential initialization
  - Property package
  - Hydrodynamics
  - Mass balance
  - Energy balance
  - Solve full system



Moving Bed

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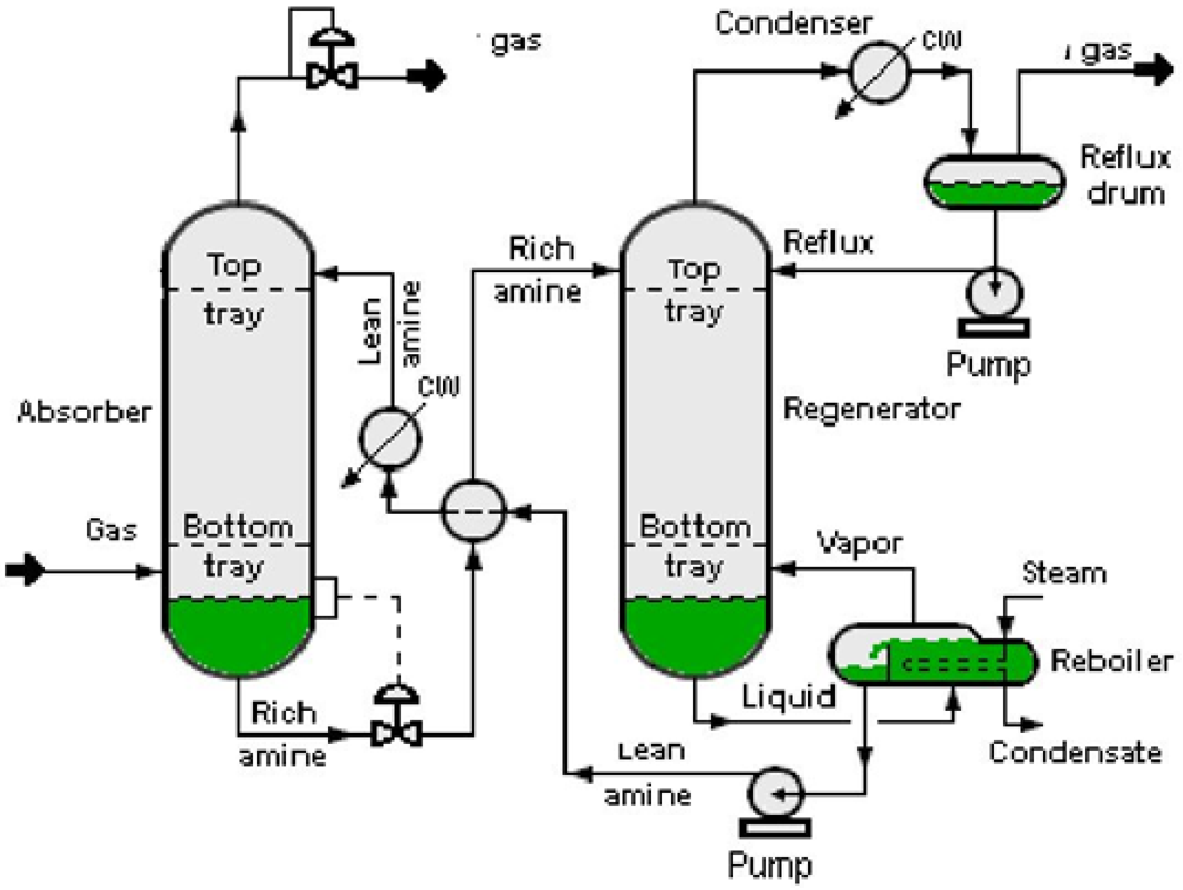
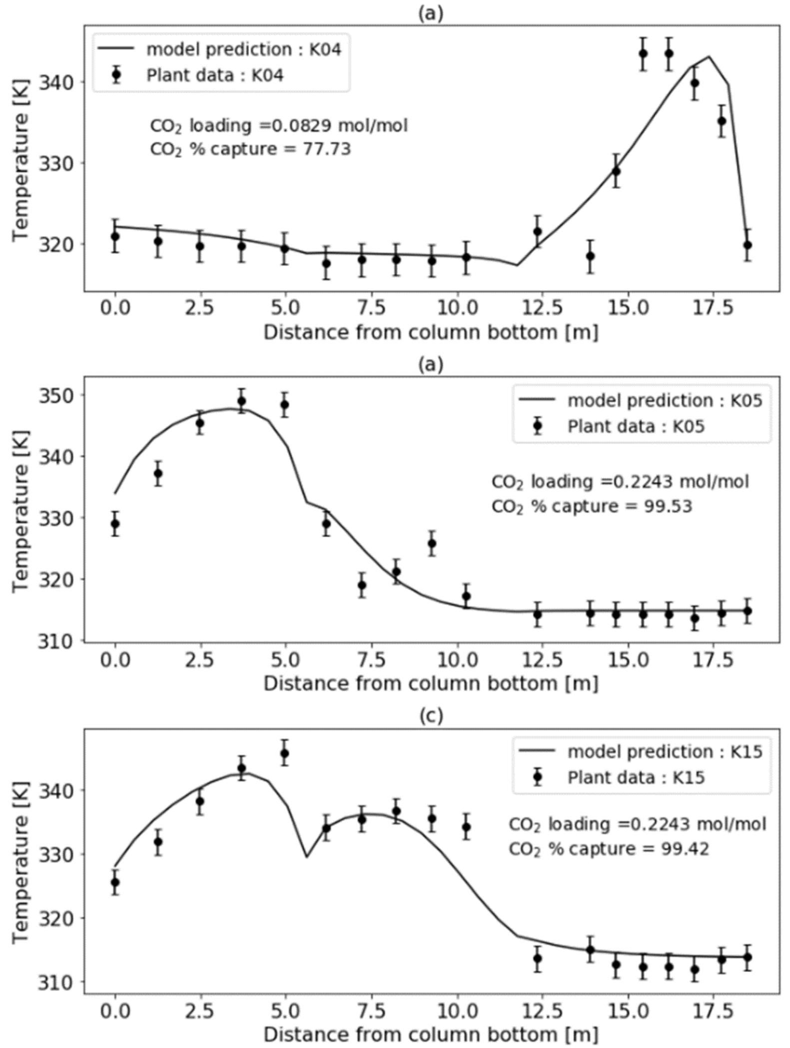
Dynamic, Two-Film Tower Model for an Electrolyte System





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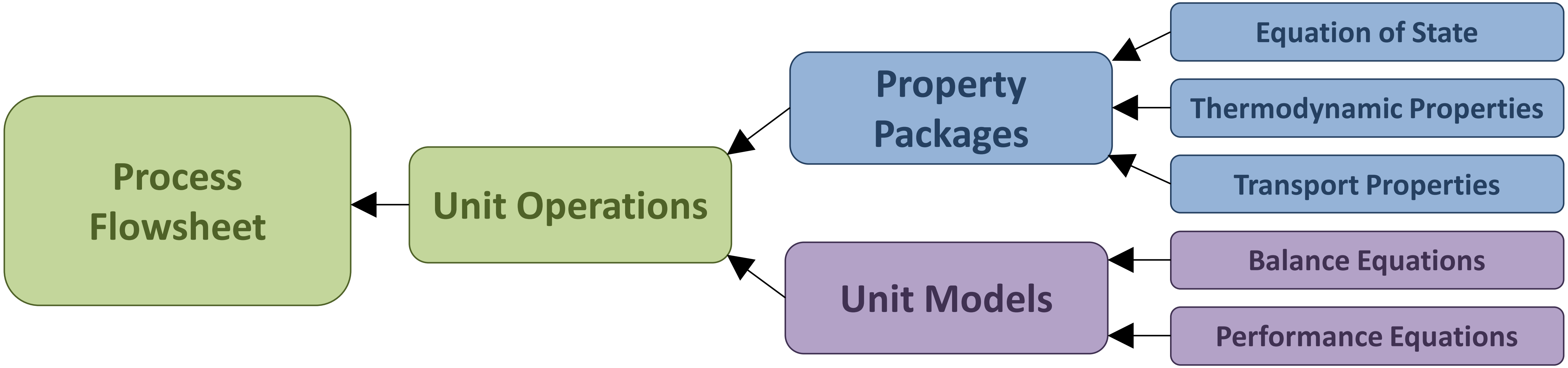
Core IDAES Framework Development

- **First public release: Github**

- **“Structured AML” – combines features of process simulators and AMLs**



- Flexible, modular framework allows for models with different levels of rigor and complexity

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