The Institute for the Design of Advanced Energy Systems (IDAES)


* National Energy Technology Laboratory, b Lawrence Berkeley Laboratory, c Sandia National Laboratories, d Carnegie Mellon University, d West Virginia University

Overview
- Next generation modeling and optimization platform
- Flexible and open model
- Complete provenance information
- Supports advanced solvers and computer architecture
- Intrinsic UQ
- Process Synthesis, Integration, and Intensification
- Process Control and Dynamics
- Apply to development of novel energy systems
- Chemical Looping
- Oxy-combustion
- Transformational Carbon Capture
- Not intended to compete with commercial simulators
- Intended to be
  - National Lab and University Capability
  - Open Source
  - Builds on knowledge gained from CCSI

Vision
- Process Dynamics and Process Control
- Process Optimization
- Identifying New Advanced Energy Concepts
- Analysis of Energy Systems
- Understand Data Requirements
- Investigate Multiple Scenarios across Time and Length Scales
- Data Management: Data, Provenance, Organize Models, Link Scales/Tasks
- Inherently Dynamic Systems – Design & Control
- Solvers and Computational Platform to Enable Solution of Large Scale Problems
- Incorporation and Assessment of Uncertainty Across Models/Scales

Projects
- 2.1. Advanced Optimization Strategies for Bubbling Fluidized Bed Larry Biegler, Mingzhao Yu, David Molina Thierry
- 2.2 Advanced Oxycombustion Systems Optimization Larry Biegler, John Eason, Jinliang Ma
- 2.3 Chemical Looping Systems Optimization Andrew Lee, TBD
- 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
- 2.6 Advanced Solvent System Optimization John Eslick, Debangsu Bhattacharyya, Paul Akula
- 2.7 Conceptual Design Tools Ignacio Grossmann, Qi Chen, John Sirola

3. Software Architecture, Algorithms, and Distributed Computing
- 3.1 System Architecture John Sirola, Dan Gunter
- 3.2 Optimization Algorithms and Parallel Computing Nick Sahinidis, Benjamin Sauk, Dan Gunter, John Sirola
- 3.3 Data Management and Workflow Deb Agarwal, You-Wei Cheah

Data Management Framework (DMF)
- Github repository for model software
- Pyomo
  - Modeling language selected for IDAES
  - Developed at Sandia National Lab
  - Based on Python
  - Open Source

Parallel Computing
- Pyomo
  - Development of algorithms for parallel computing, both CPU and GPU will be explored

Chemical Looping
- Molecular Design:
- Process Design:
- Process Model Library
- Models for Specific Applications and Innovative Concepts
- Process Dynamics and Process Control
- Process Optimization
- Conceptual Design
- Process Synthesis
- Process Integration
- Identify New Advanced Energy Concepts
- Analysis of Energy Systems
- Understand Data Requirements
- Investigate Multiple Scenarios across Time and Length Scales

Oxy-combustion
- Superstructure optimization of a complete oxy-combustion plant including CO2 compression
- Thermophysical Properties and Kinetics
- Equations of state for optimization developed with ALAMO techniques
- PVT properties based on relations to the equation of states
- Properties and Kinetics
- Superstructure optimization of a complete oxy-combustion plant including CO2 compression
- Thermophysical Properties and Kinetics
- Equations of state for optimization developed with ALAMO techniques
- PVT properties based on relations to the equation of states
- Properties and Kinetics

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Deb Agarwal, You-Wei Cheah, Andrew Lee, John Eason, Jinliang Ma, Paul Akula, Ignacio Grossmann, Richard Ihnken, Nick Sahinidis, Dan Gunter, Larry Biegler, Youwei Cheah, Qi Chen, John Eason, Marissa Engle, John Eslick, Chris Hanselman, Andrew Lee, Jinliang Ma, David Miller, Benjamin Sauk, John Sirola, David Miliana Thierry, Zach Wilson, Mingzhao Yu.