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

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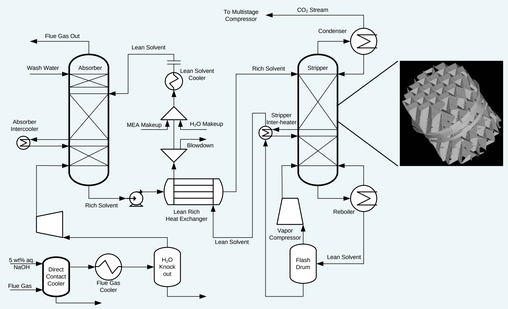
Overview

- Next generation modeling and optimization platform
  - Flexible and open model
  - Complete provenance information
  - Supports advanced solvers and computer architecture
  - Intrusive 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

Conceptual Design

- Conceptual Design and Process Integration through advanced tools for Superstructure Optimization
- Despite previous work , no general tool for Superstructure Optimization *(MIPSYN only exception)*

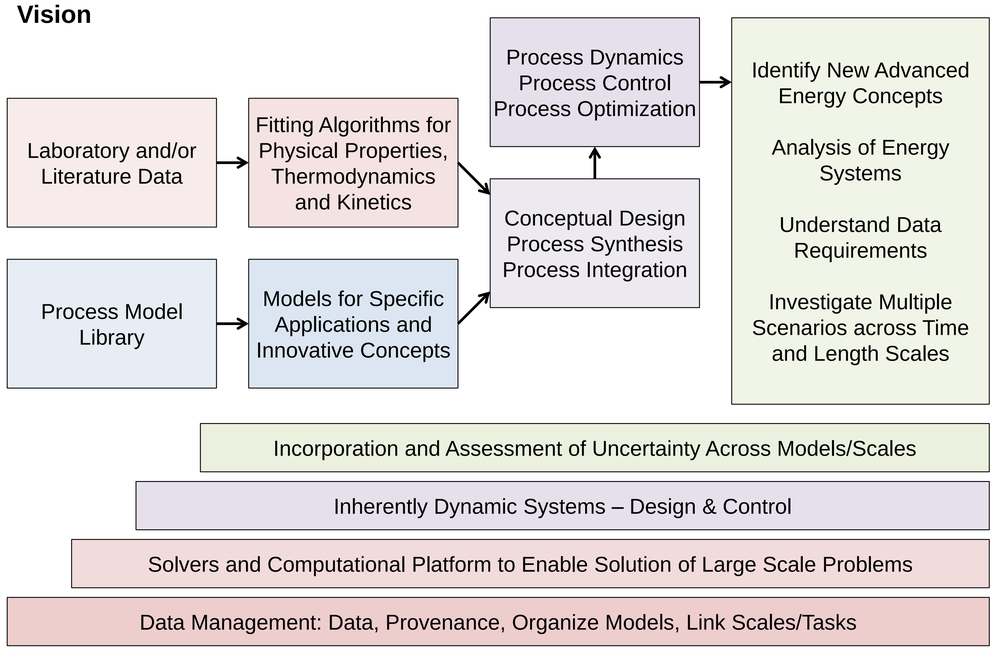
Solvents and Reactive Distillation



Contact

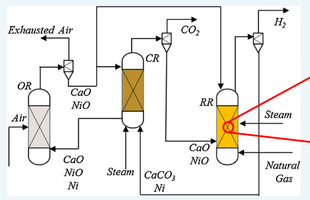
David Miller: david.miller@netl.doe.gov

Vision



Chemical Looping

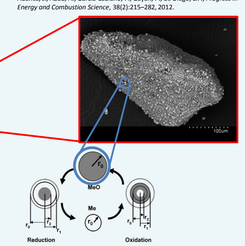
Process Design:



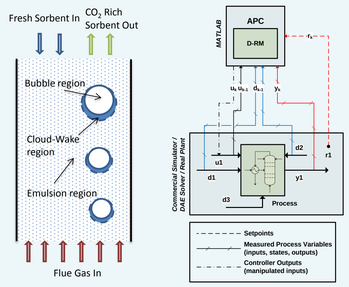
Molecular Design:

de Diego, L.F., García-Labiano, F., Gayán, P., Celaya, J., Palacios, J. M., Adánez, J., *Fuel*, 86(7-8):1036–1045, 2007.

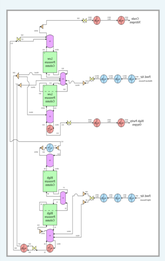
Adanez, J., Abad, A., Garcia-Labiano, F., Gayan, P., de Diego, L.F., *Progress in Energy and Combustion Science*, 38(2):215–282, 2012.



BFB, Advanced Optimization

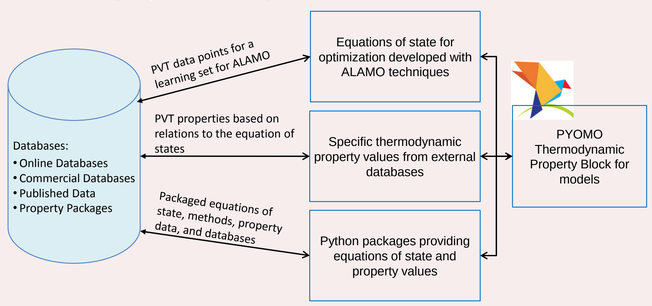


Oxy-combustion



Superstructure optimization of a complete oxy-combustion plant including CO_2 compression

Thermophysical Properties and Kinetics



Projects

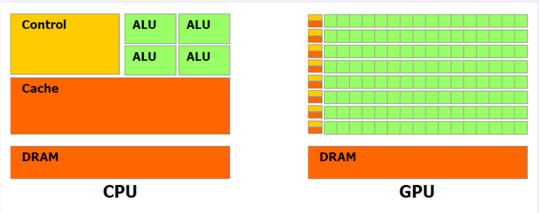
2. **Advanced Energy Systems**: Conceptual Design, Optimization, UQ, and Intensification
   - 2.1. Advanced Optimization Strategies for Bubbling Fluidized Bed
     Larry Biegler, Mingzhao Yu, David Molina Thierry
   - 2.2 Advanced Oxycombustion Systems Optimization
     Larry Biegler, John Eason, Jinliang 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 Siirola
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

Software

PYOMO

Pyomo
- Modeling language selected for IDAES
- Developed at Sandia National Lab
- Based on Python
- Open Source

Parallel Computing



Development of algorithms for parallel computing, both CPU and GPU will be explored

Data Management Framework (DMF)