Web-based Decision Support Software for Hybrid Energy Systems Based on the IDAES Framework

April 23, 2024

David Swensen (PI), Martin Denison, Corey Smithson, Aaron Felix, Markus Martin, Hong-Shig Shim, Jeff Bennett*, Nate Holwerda*, Jonathan Ogland-Hand*

Reaction Engineering International and Carbon Solutions LLC*

2024 FECM/NETL Spring R&D Project Review Meeting

For Energy and Environmental Solutions

REACTION ENGINEERING INTERNATIONAL

189 Fort Union Boulevard, Suite 201
Midvale, UT 84047
U.S.A.

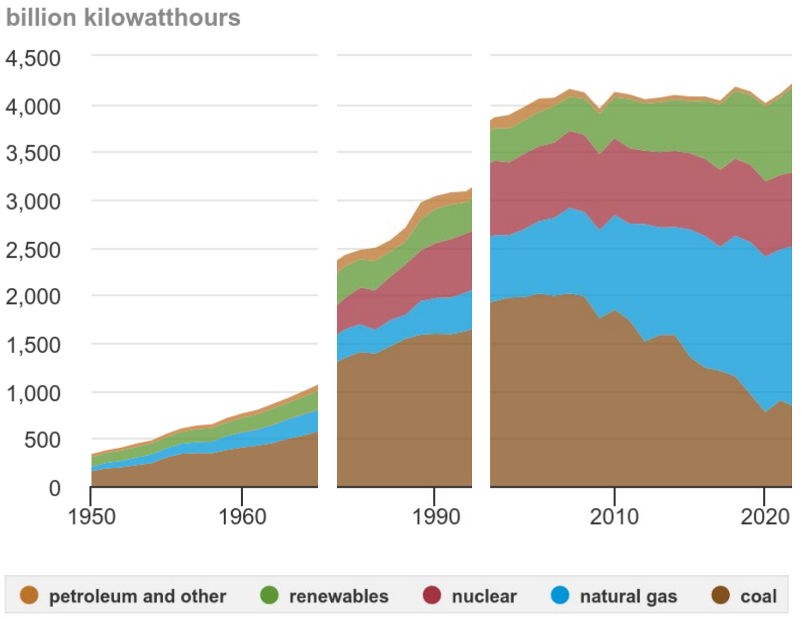
Outline

- Motivation
- Project Overview
- Technical Objectives
- Work in Progress
  - Web-based UI Framework: UI/UX
  - Hybrid Energy Decision-Support Software Architecture
  - High-Fidelity Modeling Interface
  - Other Model Development
- Concluding Remarks

Motivation

- More than 50% of US electricity production still comes from fossil fuels
- To meet climate change mitigation goal, significant deployment of carbon capture and storage (CCS) and other enabling technologies is needed while using fossil fuels as a transitional power source
- Investments in new technologies required over the next 20 years
- Hybrid Energy Systems (HES) combine:
  - Energy sources
  - Energy storage
  - Carbon capture
- Greater flexibility and lower costs for decarbonization scenarios

US Electricity Generation by Major Energy Sources, 1950-2022

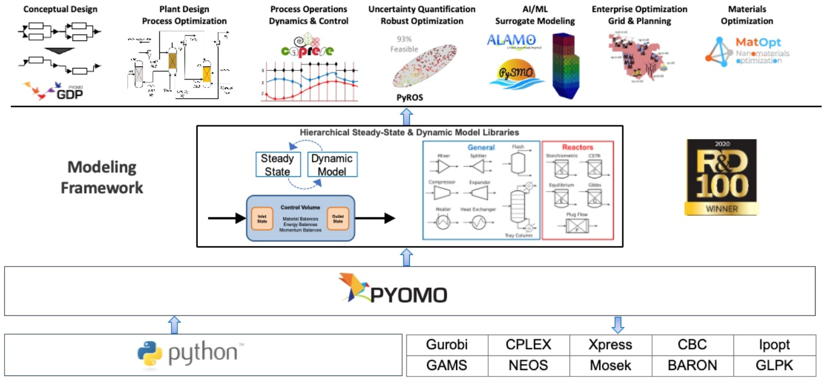


Data source: U.S. Energy Information Administration, *Monthly Energy Review* and *Electric Power Monthly* , February 2023, preliminary data for 2022
Note: Includes generation from power plants with at least 1 megawatt electric generation capacity.

IDAES Software

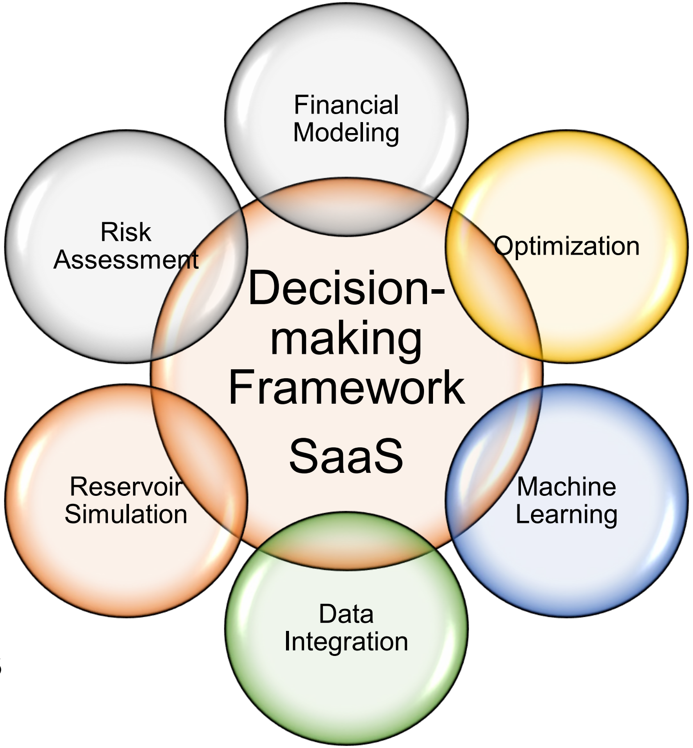
- Introduction
  - IDAES (Institute for the Design of Advanced Energy Systems)
  - Open source
  - Modeling framework for power plant and process applications
  - Equation oriented analytics
  - Dynamic analysis and optimization
  - Developed to support advanced energy systems modeling
- Challenges
  - No user interface
  - Limited models available for some aspects of hybrid energy systems
  - IDAES modeling performed using Python
  - Many energy system stakeholders and decision-makers lack the expertise to use IDAES

IDAES®
Institute for the Design of Advanced Energy Systems



Project Overview

- Goal: Facilitate transition to next generation hybrid power systems
  - Hybrid energy systems decision-making software
  - Take advantage of DOE investments
  - Expertise of REI and Carbon Solutions
- Features of decision-making software
  - Cloud-based
  - Economic analysis
  - Hybrid power systems with CCS
  - Support various decarbonization scenarios
  - Energy storage
  - Advanced user interface targets non-expert users



Funded by current and past DOE SBIR's

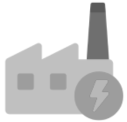
- ***Past**: "Cloud-based High-Performance Computing Decision-Making Software for Carbon Sequestration"*
- ***Current**: "Web-based Decision Support Software for Hybrid Energy Systems Based on the IDAES Framework"*

Technical Objectives

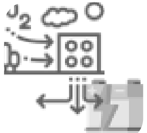
- Develop hybrid energy decision support tool
- Utilize lean development techniques to iteratively refine the software based on user feedback
  - Refine user work-flow and pre and post-processing to optimize user efficiency
  - Implement post-processing requirements
- Add additional advanced graphics and post processing abilities where applicable
- Deploy the software with a SaaS model on the cloud
- Perform extensive evaluation and testing

Hybrid Energy Decision Support Software

User Interface



Power Source Model



Energy Storage, Carbon Storage and Transport

Economic Analysis

Work Plan

- **Task 1**: Program Management and Reporting
- **Task 2**: Build Core Cloud-based SaaS Application
  - **Task 2.1**: Build Core Computational Framework Wrapper
  - **Task 2.2**: Develop Web Client Single Page Applications
  - **Task 2.3**: Back-End REST API Server Development
  - **Task 2.4**: Computing Daemon Development
- **Task 3**: Develop High-Fidelity Modeling Interface for IDAES
- **Task 4**: Integrate REI Physics-based Fireside Models Into IDAES
- **Task 5**: Develop Additional CO_2 Separation Models
- **Task 6**: Energy Storage, Carbon Transport and Storage, and Hydrogen Production and Storage
  - Task 6.1: Develop Enhanced Energy Storage Model
  - Task 6.2: Develop Carbon Transport and Storage Models
  - Task 6.3: Develop Hydrogen Production and Storage Models
- **Task 7**: Development and Integration of Economic Assessment Tools
- **Task 8**: Demonstration and Evaluation

Web-based Application

High-level representation of complex subsystem flowsheets
Ability to edit at flowsheet level for expert users
Template support for ease-of-use/reuse

Decision-Making Functionality

- Interpret complex simulation information
- Tabular data and charting
- Emphasis on costing data for stakeholder-users (feasibility, investment, policy decisions)
- 45Q tax credit calculator for sequestration offsets
- Full economic analysis for plants
- Capex, operations and management, tax credits, permitting and other information
- Available through a customizable decision panel

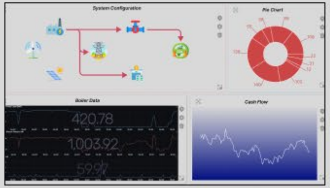
User Groups

User	Role	Key Characteristics	Scope
End-user	Decision Maker/Stakeholder /Engineer	• Usability • Results summary • Presentation quality	• Optimization • Evaluation
Configurator	Engineer	• Customizable • Modular • Flexible • Connectivity	• Objective oriented system configuration • Drag and drop, and grouping • Multi-level models: unit model, block model, island model • Optimization strategy
Developer	Engineer/Software Engineer	• Computationally Efficient • Robust • Scalable • Flexible	• Software architecture/structure • Unit model • Multi-level views • CFD-process interface • Data transfer • Widgets


PowerGen Expert
Email or ID
Password
Powered By
IDAES
REACTION ENGINEERING INTERNATIONAL

PowerGen Expert

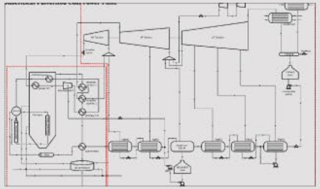
Load Decision Panel



Available Decision Panel

- *Oxyfiring with Biomass*
- *Carbon Credit Market*

System Configuration



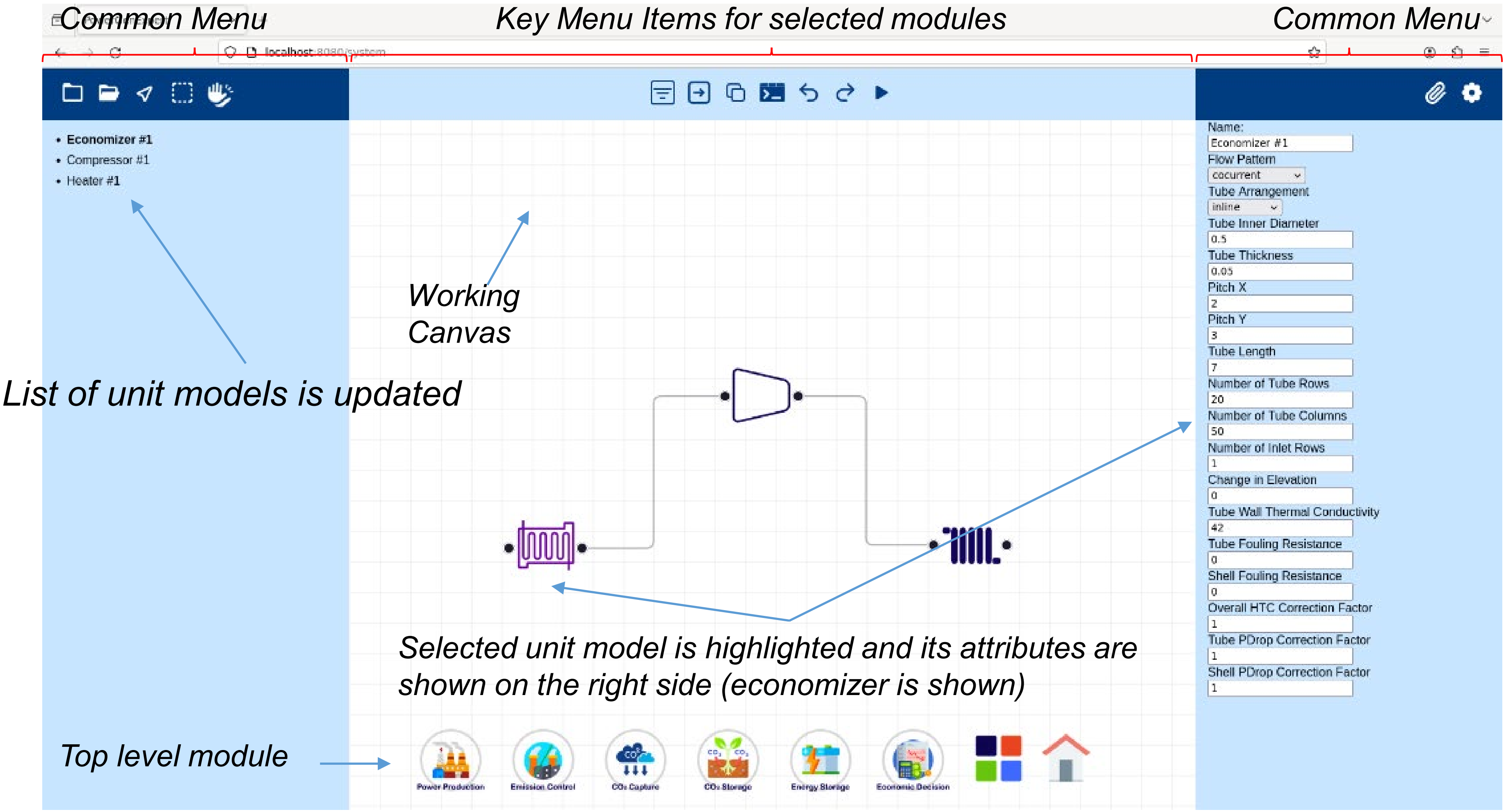
Available System Flowsheet

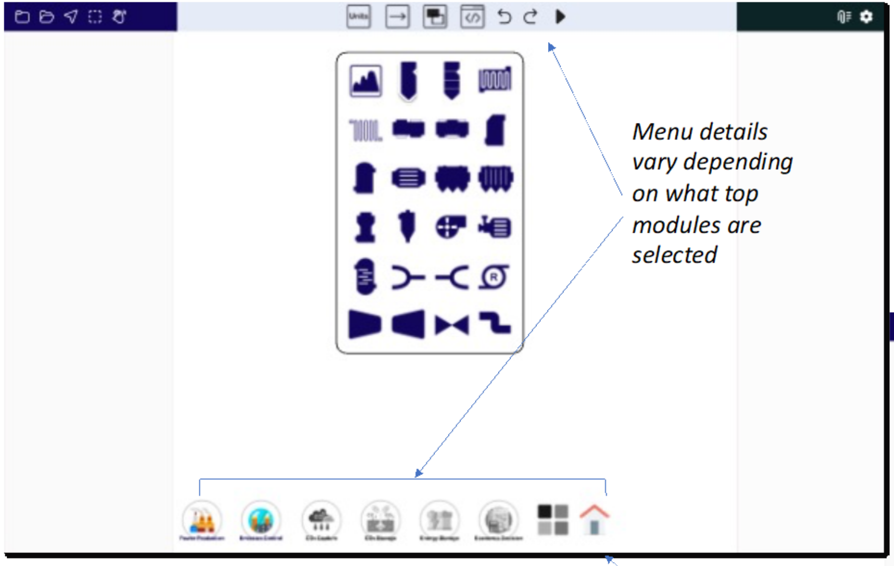
- *Subcritical Unit 300 MWe*
- *Supercritical Unit 300 MWe*
- *PacifiCorp Hunter 3*

IDAES Institute for the Design of Advanced Energy Systems

REACTION ENGINEERING INTERNATIONAL


PowerGenExpert
localhost:8080
PowerGen Expert
Power Production
Emission Control
CO_2 Capture
Economic Decision
Energy Storage
CO_2 Storage
IDAES
REACTION ENGINEERING INTERNATIONAL
System Configuration ...
Optimization / Evaluation ...

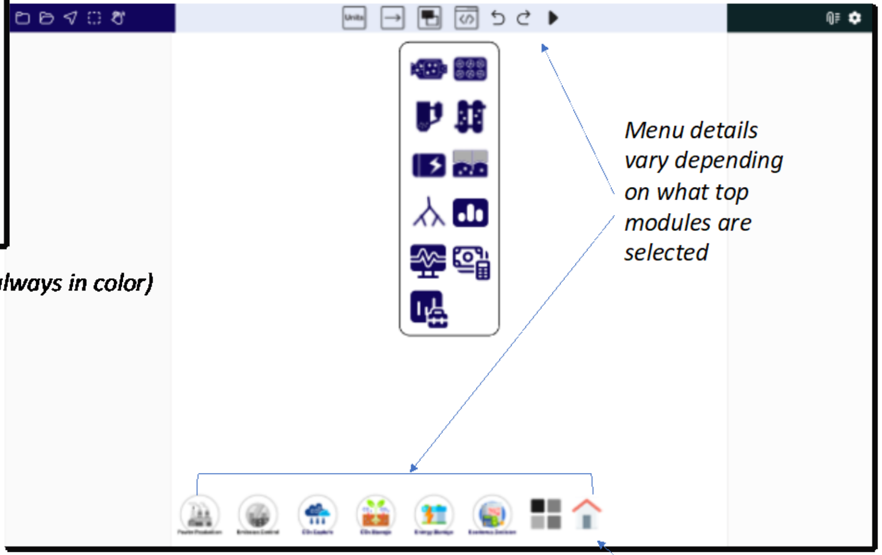

Common Menu
Key Menu Items for selected modules
Common Menu
localhost:8080/system
Economizer #1
Compressor #1
Heater #1
Working Canvas
List of unit models is updated
Name:
Economizer #1
Flow Pattern
cocurrent
Tube Arrangement
inline
Tube Inner Diameter
0.5
Tube Thickness
0.05
Pitch X
2
Pitch Y
3
Tube Length
7
Number of Tube Rows
20
Number of Tube Columns
50
Number of Inlet Rows
1
Change in Elevation
0
Tube Wall Thermal Conductivity
42
Tube Fouling Resistance
0
Shell Fouling Resistance
0
Overall HTC Correction Factor
1
Tube PDrop Correction Factor
1
Shell PDrop Correction Factor
1
Selected unit model is highlighted and its attributes are shown on the right side (economizer is shown)
Top level module
Power Production
Emission Control
CO₂ Capture
CO₂ Storage
Energy Storage
Economic Decision



Menu details vary depending on what top modules are selected

Selected top modules are in color

This is home button (always in color)



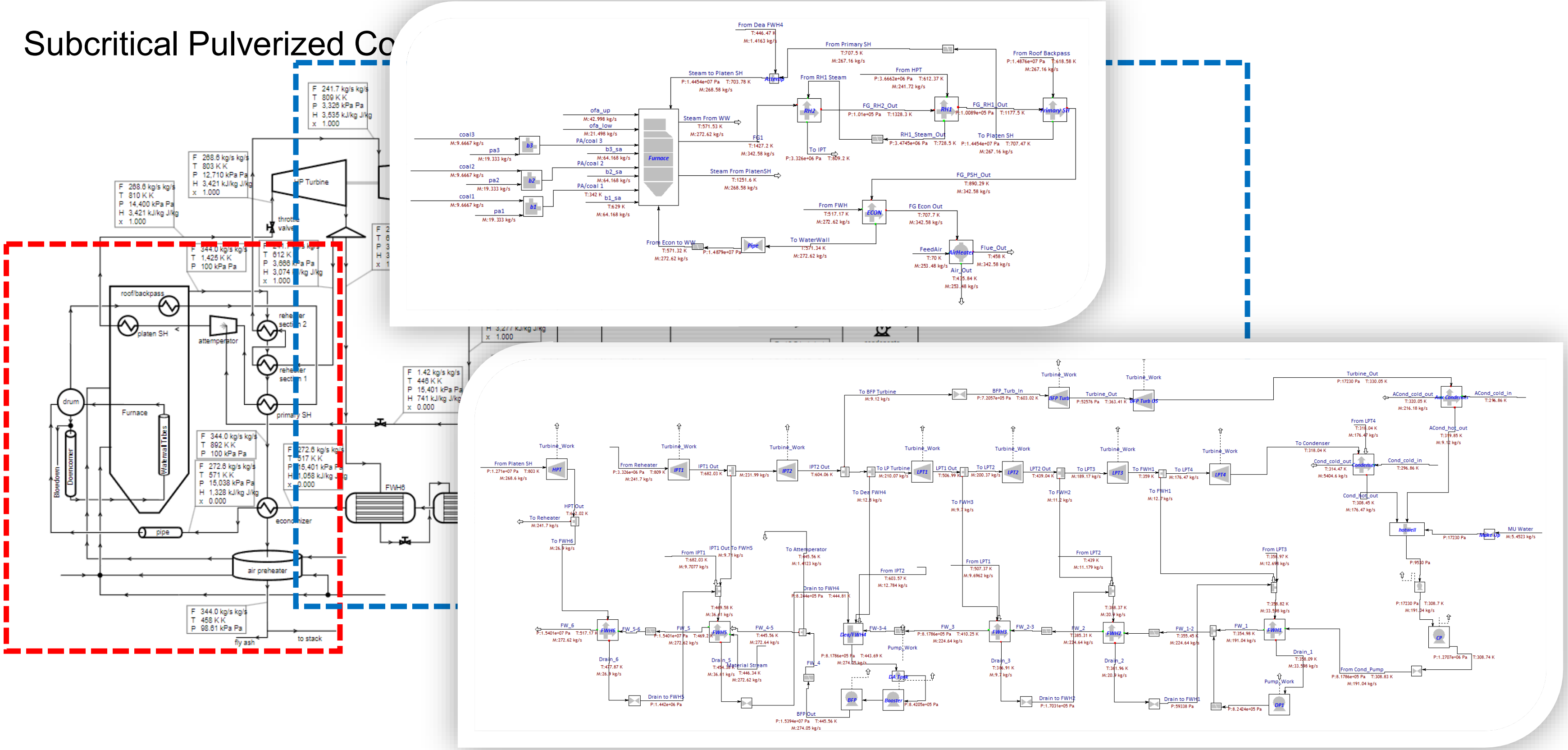
Menu details vary depending on what top modules are selected

Selected top modules are in color

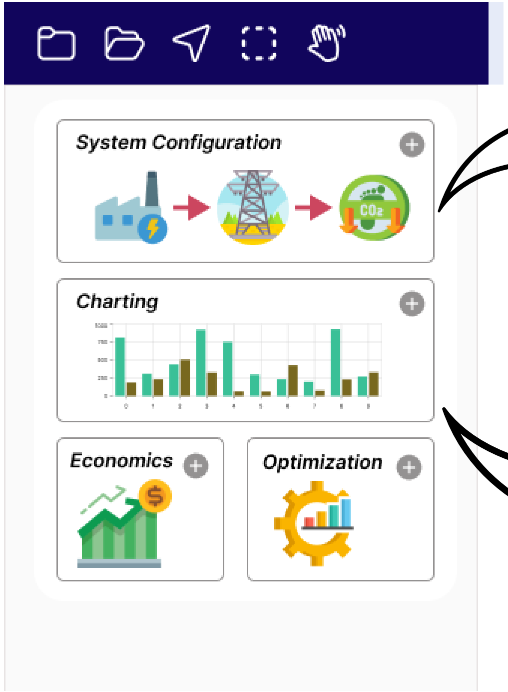
This is home button (always in color)

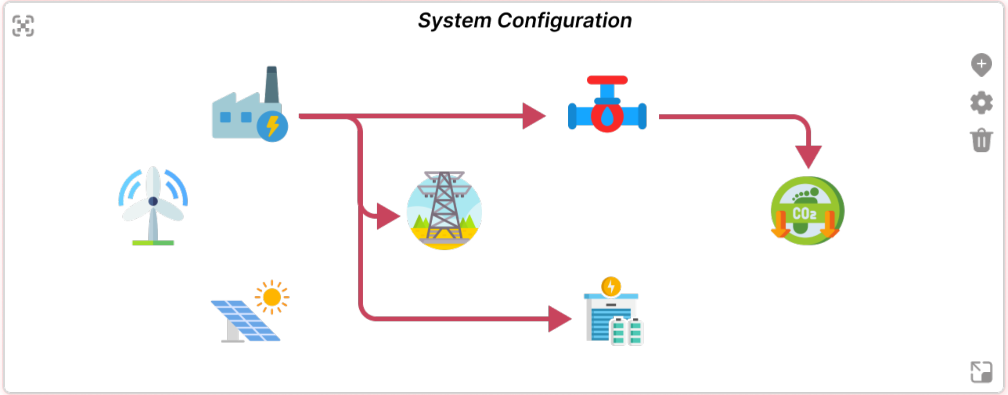
Flowsheet Template

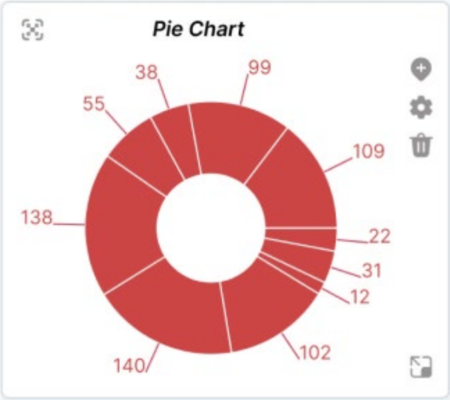
Subcritical Pulverized Co

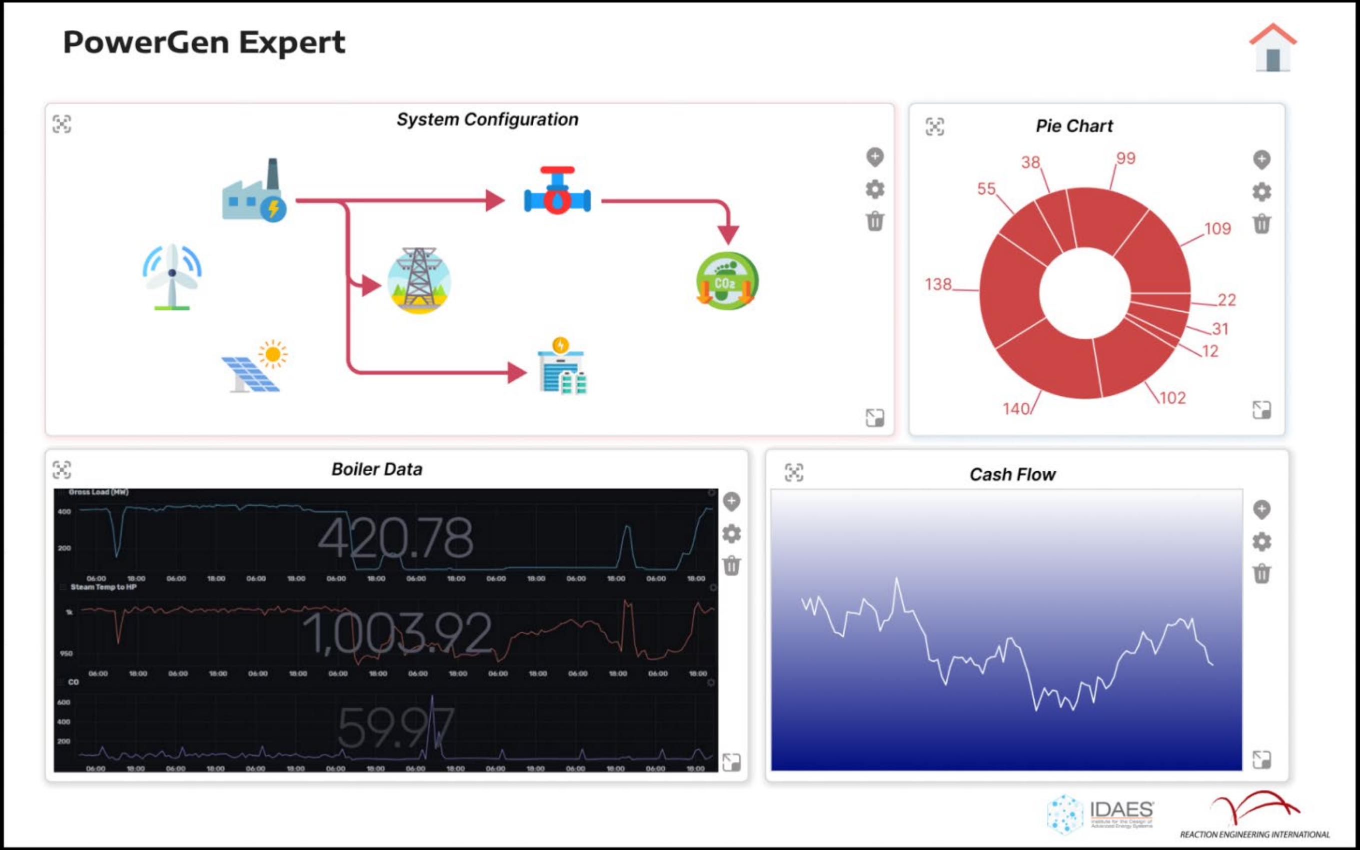


Decision Panel through Widgets

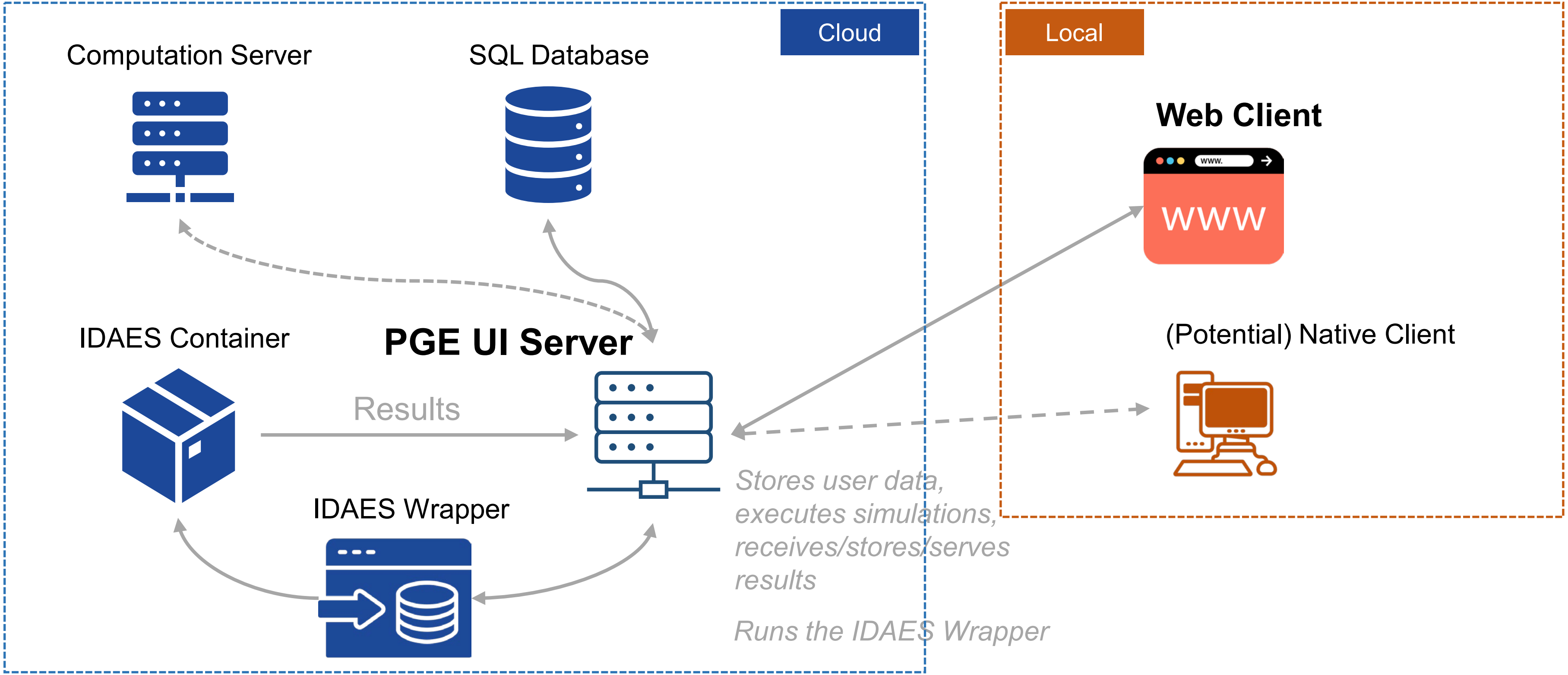




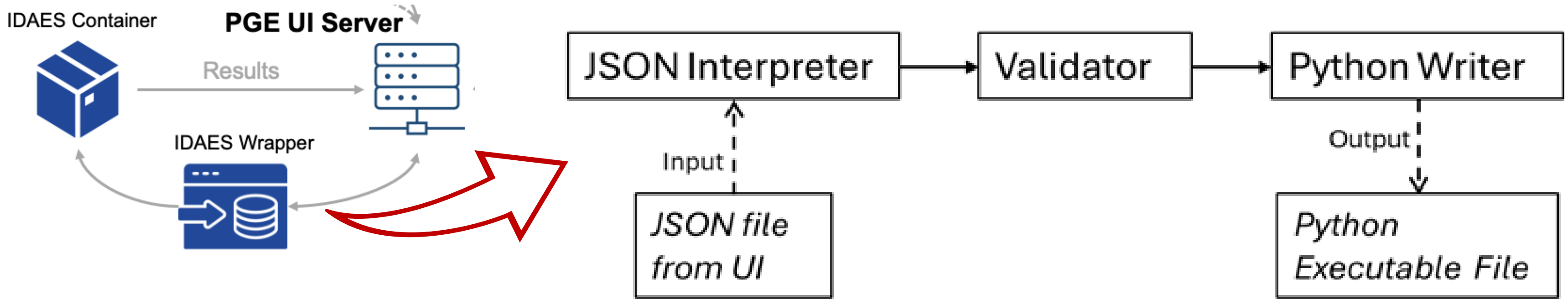



PowerGen Expert
System Configuration
Pie Chart
38
99
55
109
138
22
31
12
140
102
Boiler Data
Gross Load (MW)
420.78
Steam Temp to HP
1,003.92
CO
59.97
Cash Flow
IDAES
REACTION ENGINEERING INTERNATIONAL

UI Overall Architecture



Core Computational Wrapper



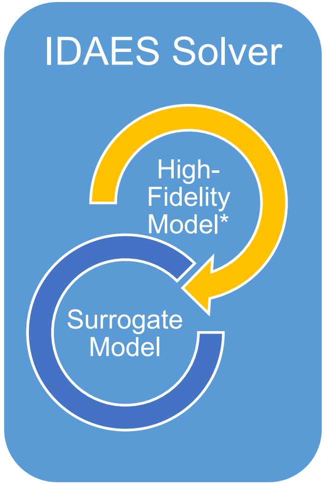
- IDAES will serve as the core computational framework
- IDAES Wrapper provides a standardized software interface to interact with IDAES
  - It accepts JSON file, perform error checking, and return a Python executable file
  - The executable file include instantiation of unit models, connecting models, defining parameters, and solving of the system
- PGE UI server runs the IDAES Wrapper with JSON System Configuration input and Python output passed to IDAES Containers for simulation execution

Web Client

- Single Page Application (SPA)
  - Loaded into the user’s web browser upon logging in the PowerGen Expert url
  - All of the codes is loaded only once
  - Further user interaction similar to the use of a native desktop application with the occasional server call
- Potential future development of Native Client

High-Fidelity Modeling Interface for IDAES

- Create an interface of a high fidelity CFD furnace fireside model with IDAES
- Our approach is to provide the sensitivity involving direct single solutions (no sensitivity calculated for a given solve)
  - Perturbations applied separately to each input variable of the input parameter point
  - The furnace surrogate representation is expressed as a linear Taylor series expansion where an expansion matrix is obtained from finite differences
  - Small Perturbation lets each run converge faster than runs from scratch
- Linear surrogate approach with sensitivity matrix is used to minimize the number of required CFD calculations
- In parallel, REI's fast running multizone furnace model based on first principles is used
  - Output data will be fed to an AI package to create the nonlinear surrogate representation automatically integrated into IDAES
  - Multiple artificial intelligence-based machine learning approach will be utilized to facilitate rapid model identification and evaluation
- Will greatly simplify the user's involvement in creating the surrogate



* Or fast running first principle model

CFD Model Inputs and Outputs for Surrogate Fit

Surrogate Inputs

1	Solid fuel flow rate
2	Fraction Biofuel
3	Primary air to coal ratio
4	Coal water mass frac
5	Stoichiometirc ratio lower furnace
6	Overall Stoichiometric Ratio
7	Secondary air temperature
8	Platen SH temperature
9	Biofuel water mass frac
10	Roof wall temperature

Surrogate Outputs

1	Water wall duty (W)
2	Platen SH duty (W)
3	Roof duty (W)
4	Carbon in ash
5	NOx (ppmw)

5 x 10 Sensitivity Matrix, A, For CFD

Linear surrogate for CFD:

$$\varphi_{output} = \varphi_0 + A\nabla\varphi_{input}$$

Each linear representation has a region of validity. If solution point, φ_{output}, is outside the region, then a new CFD surrogate linear fit is created.

MZ Furnace Model Inputs and Surrogate Fit

	Surrogate Inputs	Number of Input Values for Training
1	Solid fuel flow rate	5
2	Primary air to coal ratio	2
3	Coal water mass frac	4
4	Stoichiometirc ratio lower furnace	4
5	Overall Stoichiometric Ratio	4
6	Secondary air temperature	5
7	Platen wall temperature	4
8	Roof wall temperature	4

$$N_{Cases\ for\ Training} = \prod_{i}^{N_{surrogate\ inputs}} N_{values,i} = 51{,}200$$

Physics-based Fireside Models

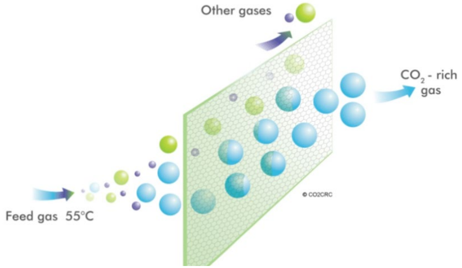
Use REI expertise to develop advanced boiler models for IDAES

- Develop and integrate surrogate dictionaries based on first-principle models
- Calculation of the heat duty to boiler regions
- Prediction of emissions and unburned carbon in fly-ash
- Models for BECCS, hydrogen and ammonia combustion, and oxy-combustion

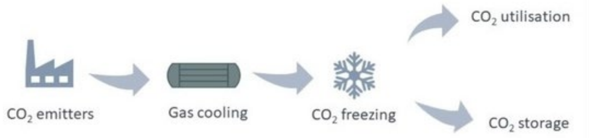
Other Model Developments

- Additional CO_2 separation model
- Energy storage, carbon transport and storage, and hydrogen production and storage
- Economic assessment tool

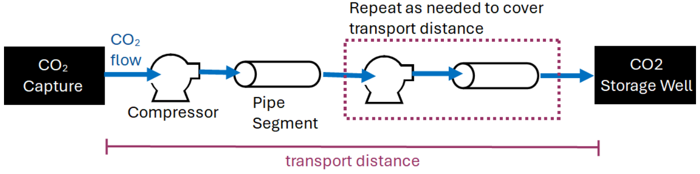
Membrane Carbon Capture



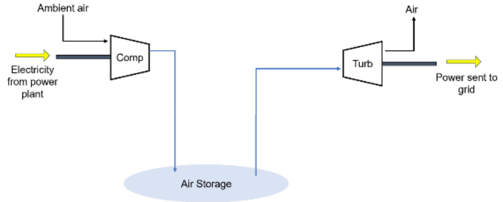
Cryogenic Carbon Capture



CO_2 Transport



Compressed Air Energy Storage (CAES)



Concluding Remarks

- Significant progress towards the project goals have been accomplished
- Core computational framework wrapper has been developed to provide a standardized software interface to interact with IDAES
- Overall structure of web-based graphical user interface that wraps together IDAES functionality along with advanced decision-making features has been developed and the details are being implemented
- User interface and user experience will be continuously refined throughout the program
- Novel approach to interface high-fidelity model with IDAES surrogate model is being developed
- Other model developments will be performed and implemented in PowerGen Expert framework with IDAES

Acknowledgements

- This material is based upon work supported by the Department of Energy Award Number DE-SC0022426
- DOE/NETL Project Manager: Mr. Omer Bakshi