IDAES
Institute for the Design of Advanced Energy Systems

Optimizing Innovative Process and Energy Systems of the Future

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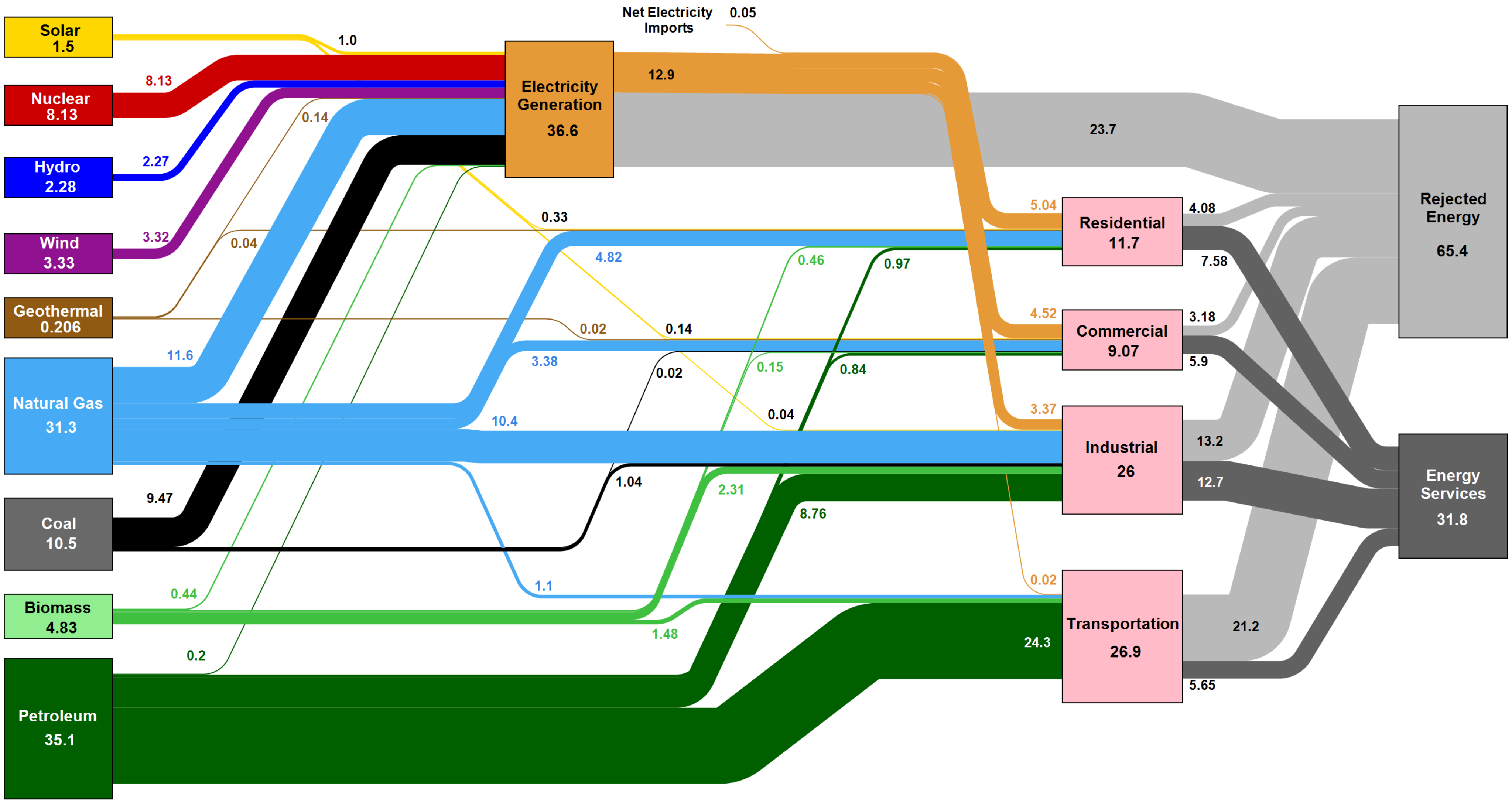
Chief Research Officer
National Energy Technology Laboratory

NATIONAL ENERGY TECHNOLOGY LABORATORY

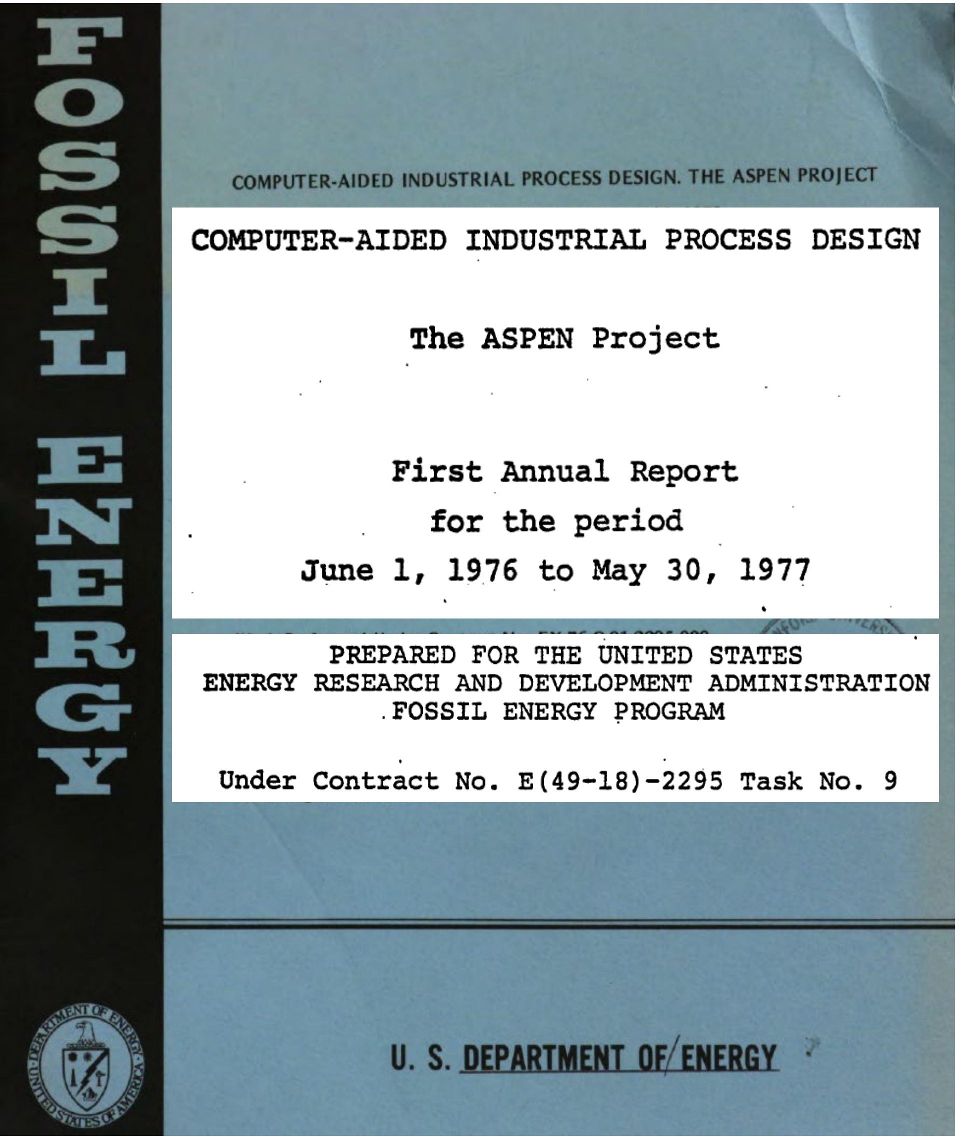
U.S. DEPARTMENT OF ENERGY

Estimated U.S. Energy Consumption in 2021: 97.3 Quads



Source: LLNL March, 2022. Data is based on DOE/EIA MER (2021). If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant heat rate. The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential sector, 65% for the commercial sector, 21% for the transportation sector and 49% for the industrial sector, which was updated in 2017 to reflect DOE's analysis of manufacturing. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

DOE/FECM History of Innovation for Decision Support Tools



FOSSIL ENERGY

COMPUTER-AIDED INDUSTRIAL PROCESS DESIGN. THE ASPEN PROJECT

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

U. S. DEPARTMENT OF ENERGY

MFiX

CCSI
Carbon Capture Simulation Initiative

CCSI²
Carbon Capture Simulation for Industry Impact

IDAES
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DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

NAWI
National Alliance for Water Innovation

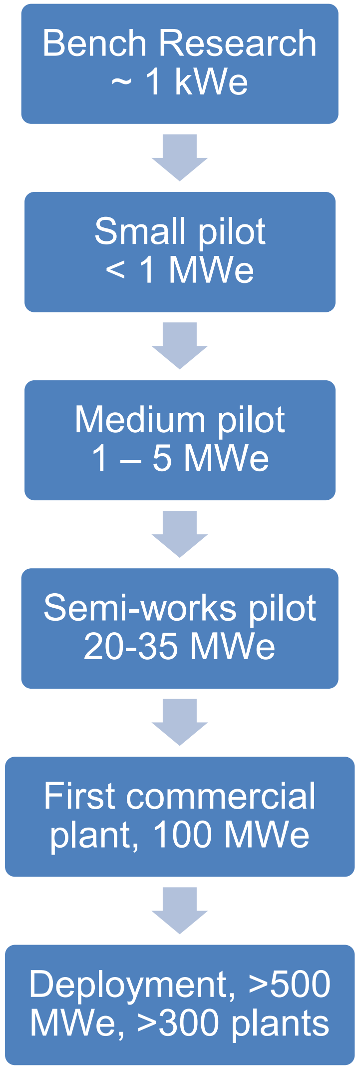
Water TAP

PARETO
The Produced Water Optimization Initiative

PrOMMiS

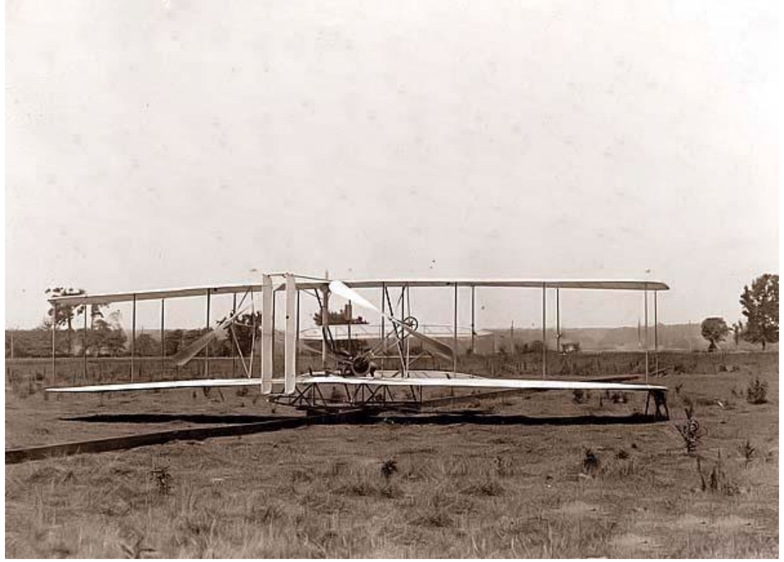
Carbon capture challenge

- The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades
- President [Obama]'s plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years
- To help realize the President's objectives, new approaches are needed for taking CCS concepts from lab to power plant, <u>quickly</u>, and at low cost and risk
- CCSI will accelerate the development of CCS technology, from discovery through deployment, with the help of science-based simulations

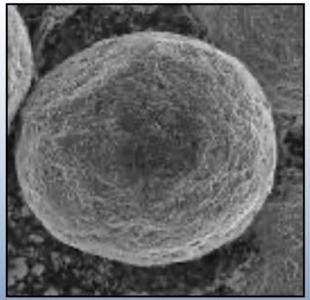


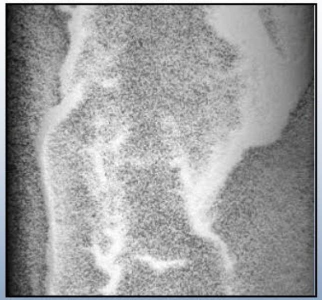
How can we accelerate technology development for carbon capture and storage?

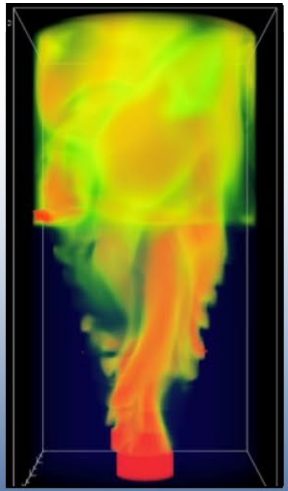
Key differences in the design process used to create these two machines:
better science, more engineers…..and also large-scale simulations



Develop M&S tools to accelerate the commercialization of CCS







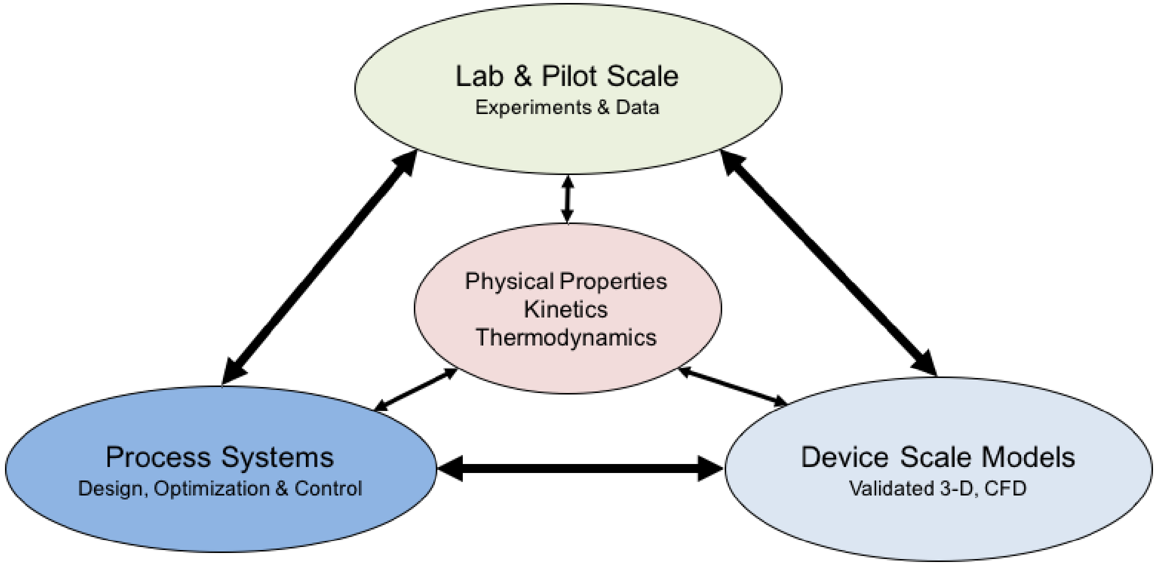
Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

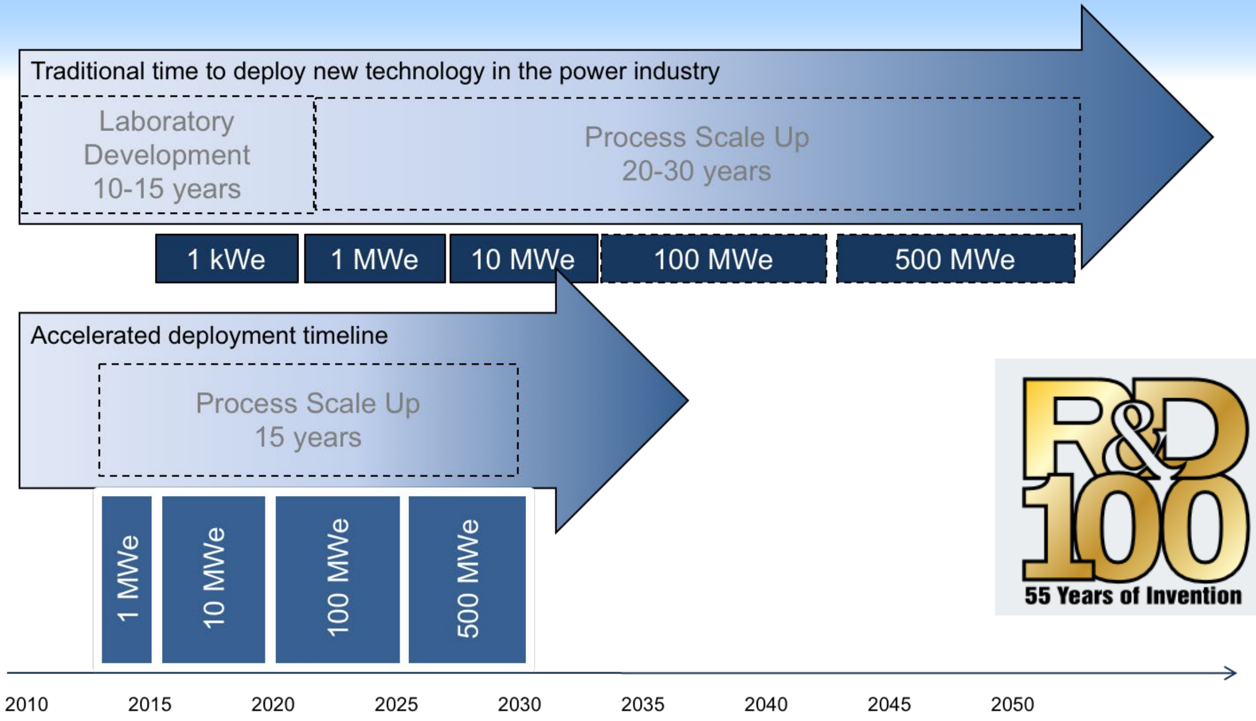
On June 28-29, 2011 CCSI Team visited Boeing's Integrated Technology Development Lab and the Everett manufacturing plant to learn how they are successfully using simulation and modeling to accelerate the development of new aircraft, such as the 787.

CCSI (2011-2016)

Carbon Capture Simulation Initiative

Maximize the learning at each stage of technology development





R&D 100 — 55 Years of Invention

Industry Collaborators

Available Open Source

https://github.com/CCSI-Toolset/

www.acceleratecarboncapture.org

Multi-disciplinary, Multi-institutional Collaboration

CCSI Carbon Capture Simulation Initiative

NETL

Berkeley Lab

Lawrence Livermore National Laboratory

Los Alamos National Laboratory EST.1943

Pacific Northwest National Laboratory

U.S. Department of Energy

CCSI^2

Carbon Capture Simulation for Industry Impact

Technology Centre Mongstad – Summer 2018

www.tcmda.com

Sequential Design of Experiments to Maximize Learning from Carbon Capture Pilot Plant Testing

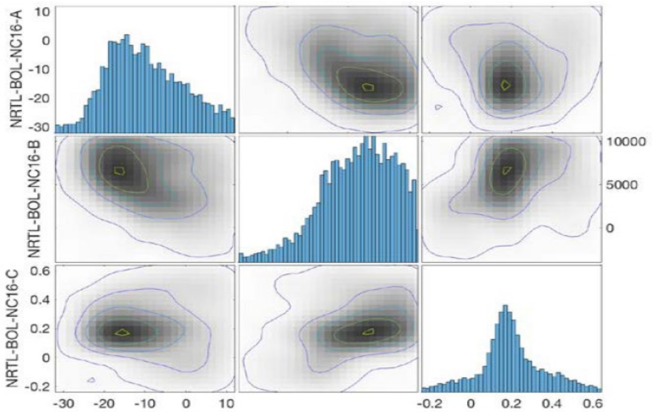
Model + Experiments + Statistics

Ensure right data is collected

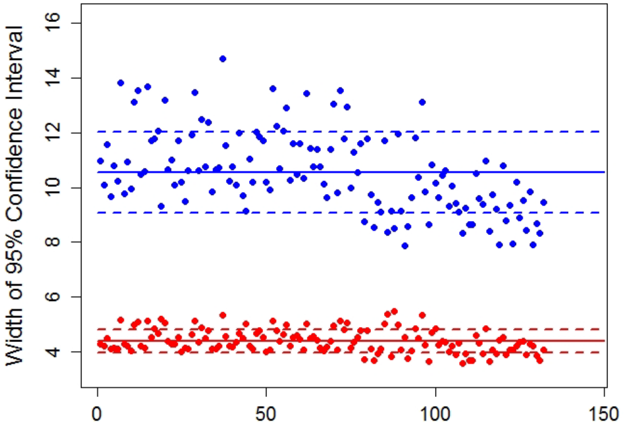
Maximize value of data collected

Technical Risk Reduction Through Simulation-Based Engineering

Uncertainty Quantification



Maximizing Learning



NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Lawrence Livermore National Laboratory

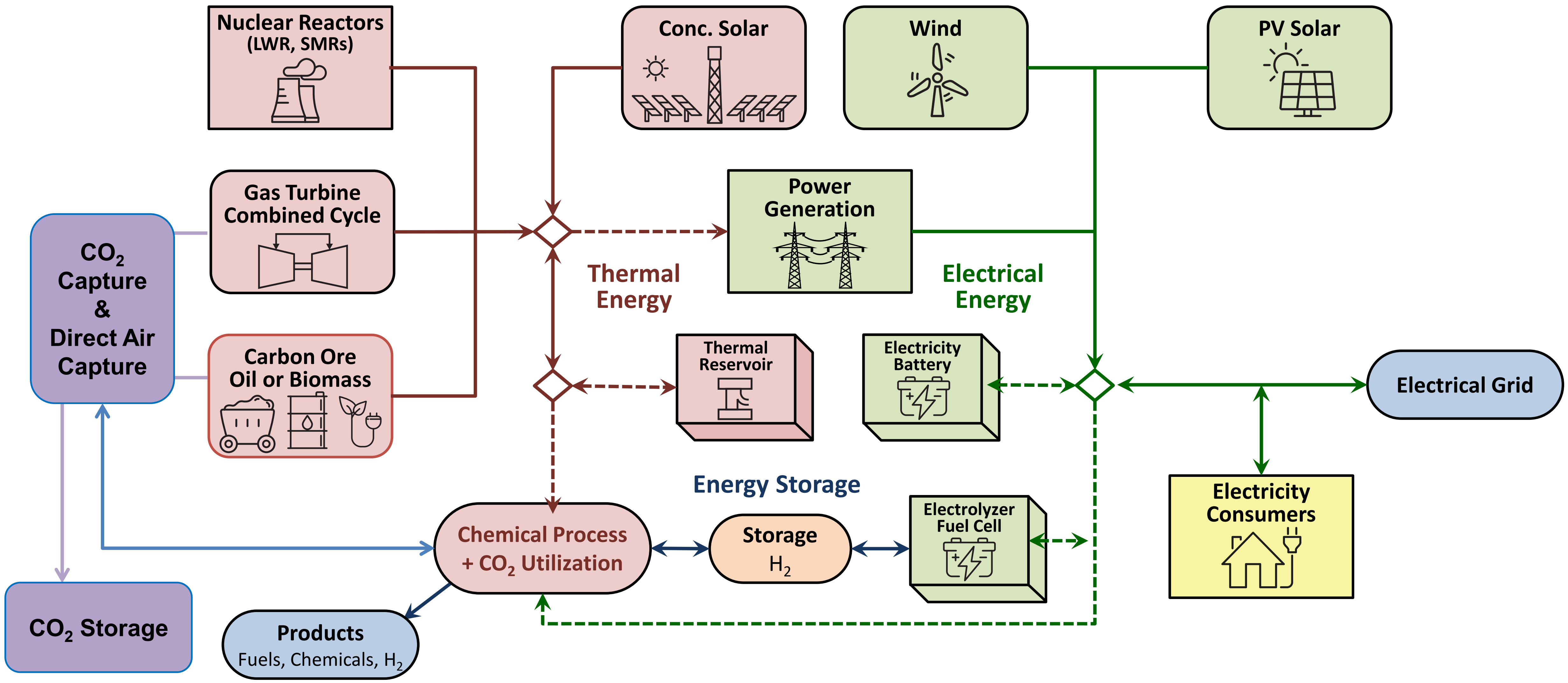
Los Alamos NATIONAL LABORATORY EST. 1943

Pacific Northwest NATIONAL LABORATORY

West Virginia University

THE UNIVERSITY OF TEXAS AT AUSTIN

Increasingly Integrated Energy & Process Systems



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Decision Making for Energy and Process Systems

Decisions

- Process operation
- Process design
- Technology selection
- R&D priorities

Approaches

- Approximations
- Heuristics
- Spreadsheets
- Simulation
- Optimization

$$\min f(x, u)$$
$$h(x, u) = 0$$

Understanding large, complex systems: Don't Simulate → Solve

Derivative-free ("black-box") optimization (DFO)
~ 100-1000 simulations

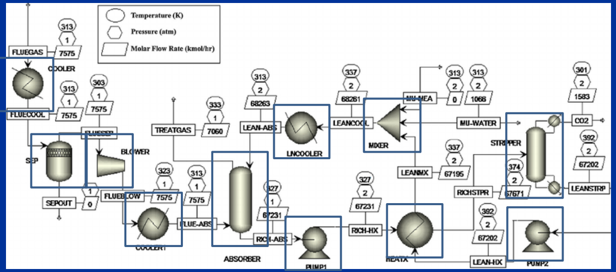
Optimization over degrees of freedom only

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

u

f

Simulator



Equation-oriented (EO) Optimization
model embedded as algebraic constraints

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

Glass-box optimization
~ 1-5 "Simulation Time Equivalents"
Leverage exact derivatives, sparse structure

[Adapted from Biegler, 2017]

Biegler, L. T., D. C. Miller and C. O. Okoli (2021). Don't Search - Solve! Process Optimization Modeling with IDAES. *Simulation and Optimization in Process Engineering: The Benefit of Mathematical Methods in Applications of the Chemical Industry*. N. Asprion and M. Bortz, Elsevier.

Next-generation multi-scale modeling & optimization framework

Fully Flexible	Model Libraries
Open Model Structure	Black Box Models
Optimization	Simulation
Dynamic	Steady-State
Conceptual Design	Case Studies
Academic	Commercial

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Institute for the Design of Advanced Energy Systems

Transcending Boundaries

Built on

python™

- High-level programming language
- Rich set of tools and libraries

PYOMO

- Open-source Python package
- Streamlined optimization modelling
- Development of numerical methods
- Interfaces with optimization solvers

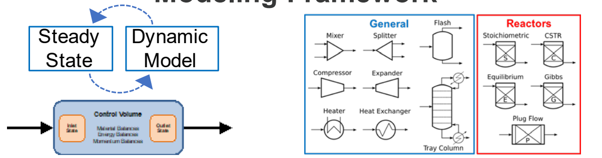
IDAES – Institute for the Design of Advanced Energy Systems

- Reusable and extensible unit models
- Equation-oriented approaches to physical property models
- Integrated with model identification and machine learning tools
- Advanced algorithms tailored to process design and optimization

IDAES Integrated Platform

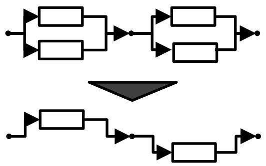
Institute for the Design of Advanced Energy Systems

Modeling Framework



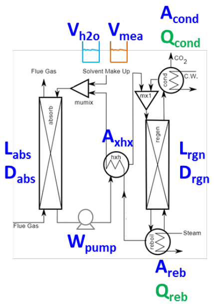
Hierarchical - Steady-State & Dynamic - Model Libraries

Conceptual Design



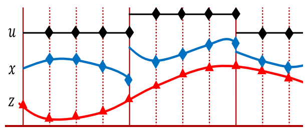
PYOMO GDP

Plant Design
Process Optimization

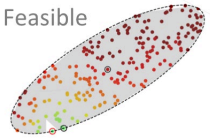


Process Operations
Dynamics & Control

caprese



Uncertainty Quantification
Robust Optimization

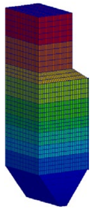


PyROS

AI/ML
Surrogate Modeling

ALAMO a black-box modeling tool

PySMO



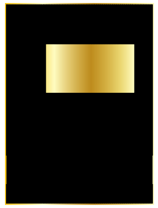
Enterprise Optimization
Grid & Planning

Materials
Optimization

MatOpt Nanomaterials optimization

Open Source: https://github.com/IDAES/idaes-pse

Lee, et al., *J. of Adv. Manufacturing and Processing* (2021)



NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Carnegie Mellon

West Virginia University

UNIVERSITY OF NOTRE DAME

Georgia Tech

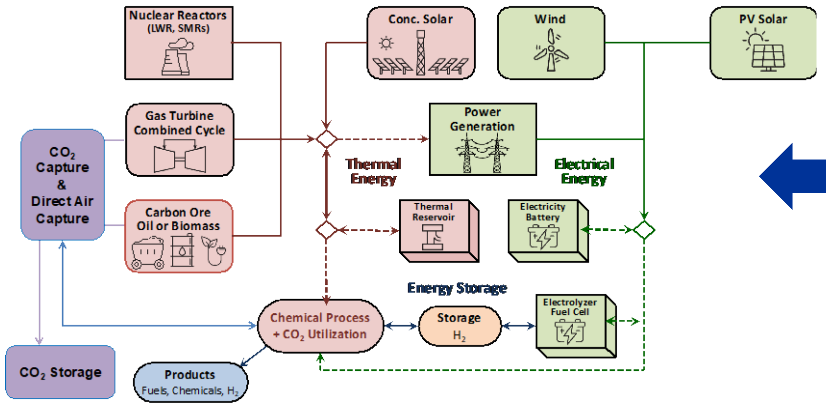
PYOMO

python™

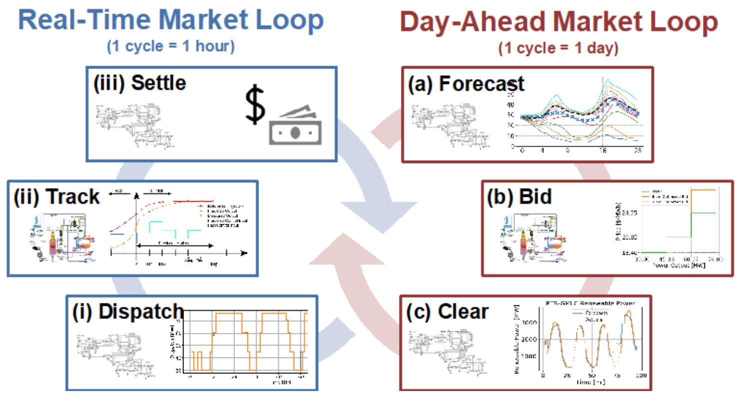
Gurobi	CPLEX	Xpress	CBC	Ipopt
GAMS	NEOS	Mosek	BARON	GLPK

Scale-Bridging to Assess Macro-scale Interactions

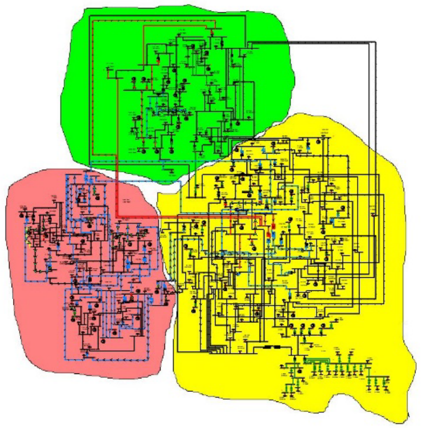
High-Fidelity Process Modeling



Integrated Resource-Grid Model



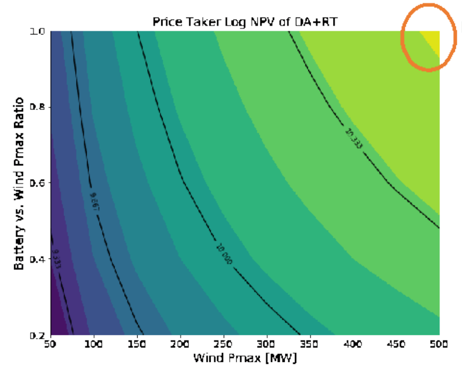
Grid Modeling



https://icseg.iti.illinois.edu/files/2013/10/IEEE118.png

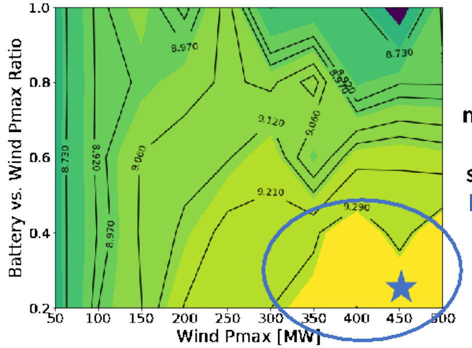
Example shows how neglecting larger interactions results in wrong conclusions.

Price-taker
contours: $\log_{10}$(NPV)



maximizes wind farm size and battery power rating

Rigorous "double loop" simulation
contours: $\log_{10}$(NPV)



maximizes wind farm size and selects modest battery power rating

Example to ***illustrate*** differences: results based on the specific grid, parameters, and control strategies that are being used

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Gao, X., B. Knueven, J.D. Siirola, D.C. Miller and A.W. Dowling (2022). "Multiscale simulation of integrated energy system and electricity market interactions." Applied Energy **316**: 119017, https://doi.org/10.1016/j.apenergy.2022.119017.

Changes in the Carbon Management Landscape

2010's

- Coal
- Baseload, steady state
- 90% Capture target

CCSI
Carbon Capture Simulation Initiative

CCSI²
Carbon Capture Simulation for Industry Impact

IDAES
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2022+

- Natural gas
- Net Zero Goals → Higher Capture Rates
  - 2035 Power Generation
  - 2050 Economy-Wide
- Flexible generation
- Large pilots & demonstration
- Industrial capture
- Carbon dioxide removal
  - Direct air capture

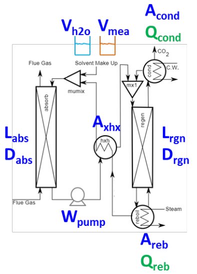
DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

Advanced Computational to Support CO_2 Capture

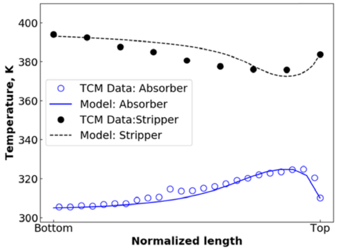
Maximizing Leaning, Reducing Technical Risk, Integrating Analysis

Rigorous Physics-Based Multiscale Stochastic Models

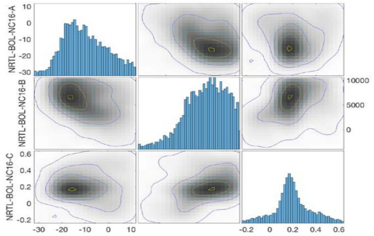
High Fidelity Process Modeling



Model Validation

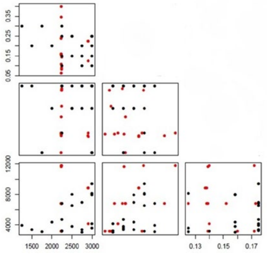


Uncertainty Quantification

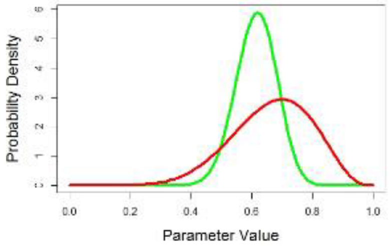


UQ Guides SDoE to Optimize Data Value, Maximize Learning

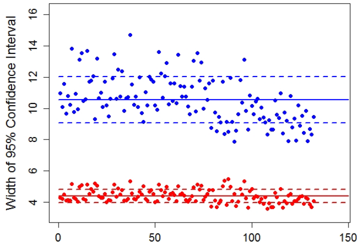
Optimize Experimental Design



Refine Model Parameters

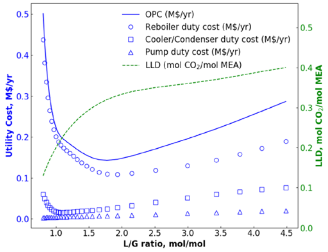


Maximizing Learning

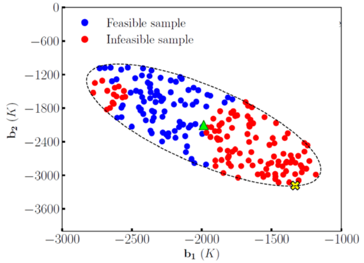


Framework for Robust-Optimal Design and Operation

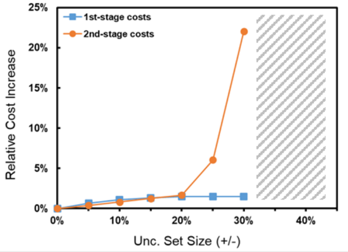
Process Optimization



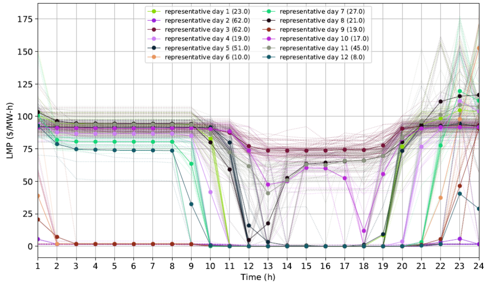
More Robust Optimal Designs

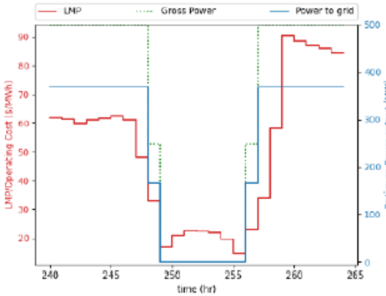


Quantify Price of Robustness



Optimizing Design & Operations for Flexible CO_2 Capture Systems





CCSI²
Carbon Capture Simulation for Industry Impact

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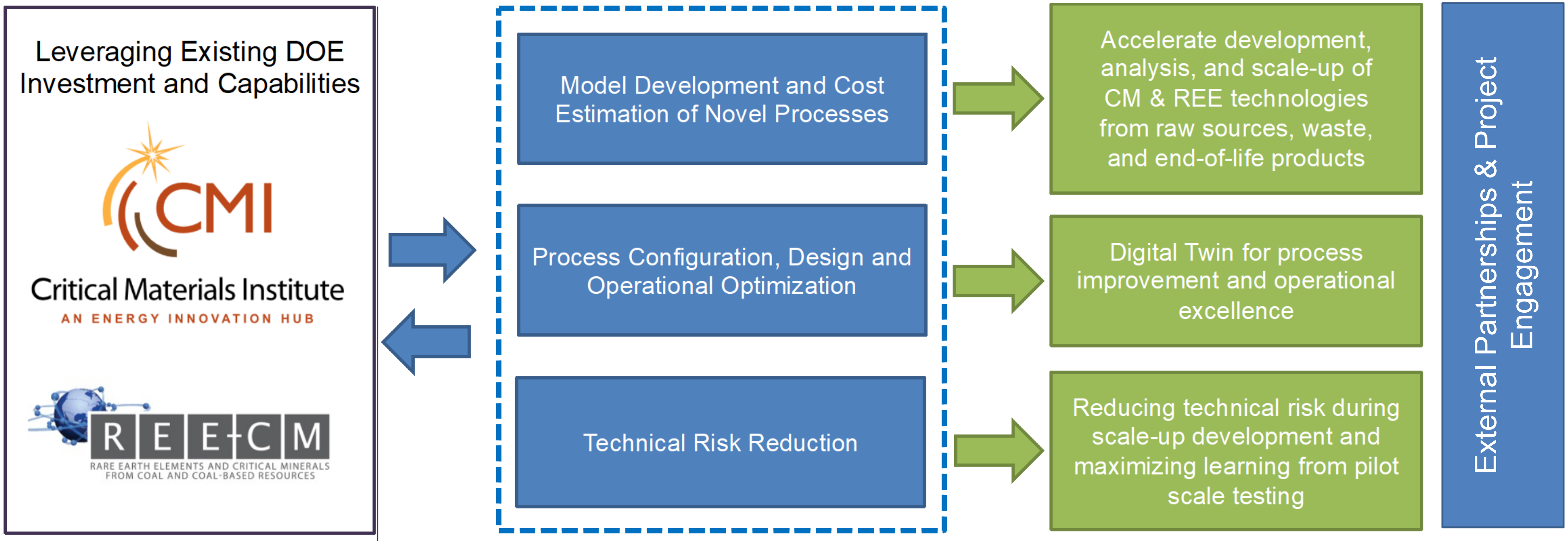
DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

Objective: accelerate identification, design, and scale-up of innovative CM & REE processes, leveraging IDAES and a decade of DOE investment and experience in CM & REE technologies.



PrOMMiS will work directly with industry and research partners to accelerate scale-up by de-risking the development and deployment of commercial-scale processes and maximizing learning in development.

Foundational Modeling and Optimization Partnerships Utilizing IDAES

Multi-lab Initiatives to Address Major National and DOE Priorities

Initiative	Focus	Partners
IDAES® Institute for the Design of Advanced Energy Systems	H_2 with Capture	National Energy Technology Laboratory; Berkeley Lab; Sandia National Laboratories; Carnegie Mellon; West Virginia University; University of Notre Dame; Georgia Tech
CCSI2 Carbon Capture Simulation for Industry Impact	Post-Combustion Carbon Capture	National Energy Technology Laboratory; Berkeley Lab; Lawrence Livermore National Laboratory; Los Alamos National Laboratory; Pacific Northwest National Laboratory; Oak Ridge National Laboratory; West Virginia University; University of Notre Dame; The University of Texas at Austin; UT; University of Pittsburgh
DISPATCHES Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems	Integrated Energy Systems	National Energy Technology Laboratory; Sandia National Laboratories; Berkeley Lab; INL Idaho National Laboratory; NREL Transforming ENERGY; University of Notre Dame
Water TAP	Water Desalination	National Energy Technology Laboratory; Berkeley Lab; NREL Transforming ENERGY; Oak Ridge National Laboratory
PrOMMiS	Rare Earth Element & Critical Mineral Recovery	National Energy Technology Laboratory; Berkeley Lab; Sandia National Laboratories; Carnegie Mellon; West Virginia University; University of Notre Dame; Georgia Tech
PARETO The Produced Water Optimization Initiative	Produced Water Management	National Energy Technology Laboratory; Berkeley Lab; Carnegie Mellon; Georgia Tech

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University of Notre Dame: Alexander Dowling, Xian Gao, Nicole Cortes
Georgia Tech: Nick Sahinidis, Yijiang Li

DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

Acknowledges support from the Grid Modernization Laboratory Consortium through FE, NE, & EERE

GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

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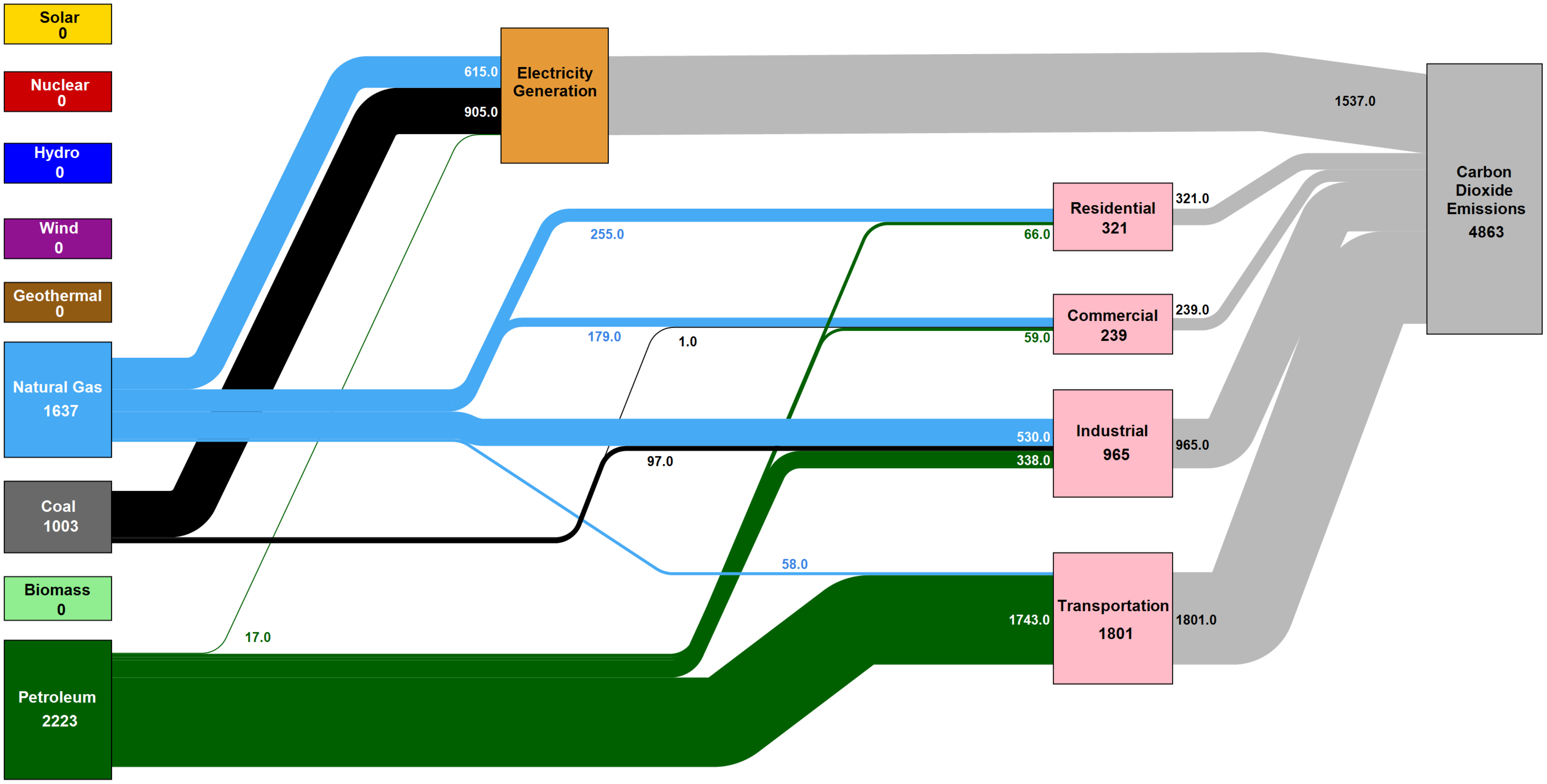
Sandia National Laboratories: John Siirola, Michael Bynum, Edna Rawlings, Jordan Jalving
Idaho National Laboratory: Cristian Rabiti, Andrea Alfonsi, Konor Frick, Jason Hansen
National Renewable Energy Laboratory: Wes Jones, Darice Guittet, Jordan Jalving, Ben Kneuven, Abinet Eseye, Ignas Satkauskas
Lawrence Berkeley National Laboratory: Dan Gunter, Keith Beattie, Oluwamayowa Amusat
University of Notre Dame: Alexander Dowling, Xian Gao

We also acknowledge support from AMO/NAWI and ARPA-E

NAWI National Alliance for Water Innovation

arpa·e CHANGING WHAT'S POSSIBLE

United States Energy-related Carbon Dioxide Emissions in 2021: 4,863 million metric tons



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