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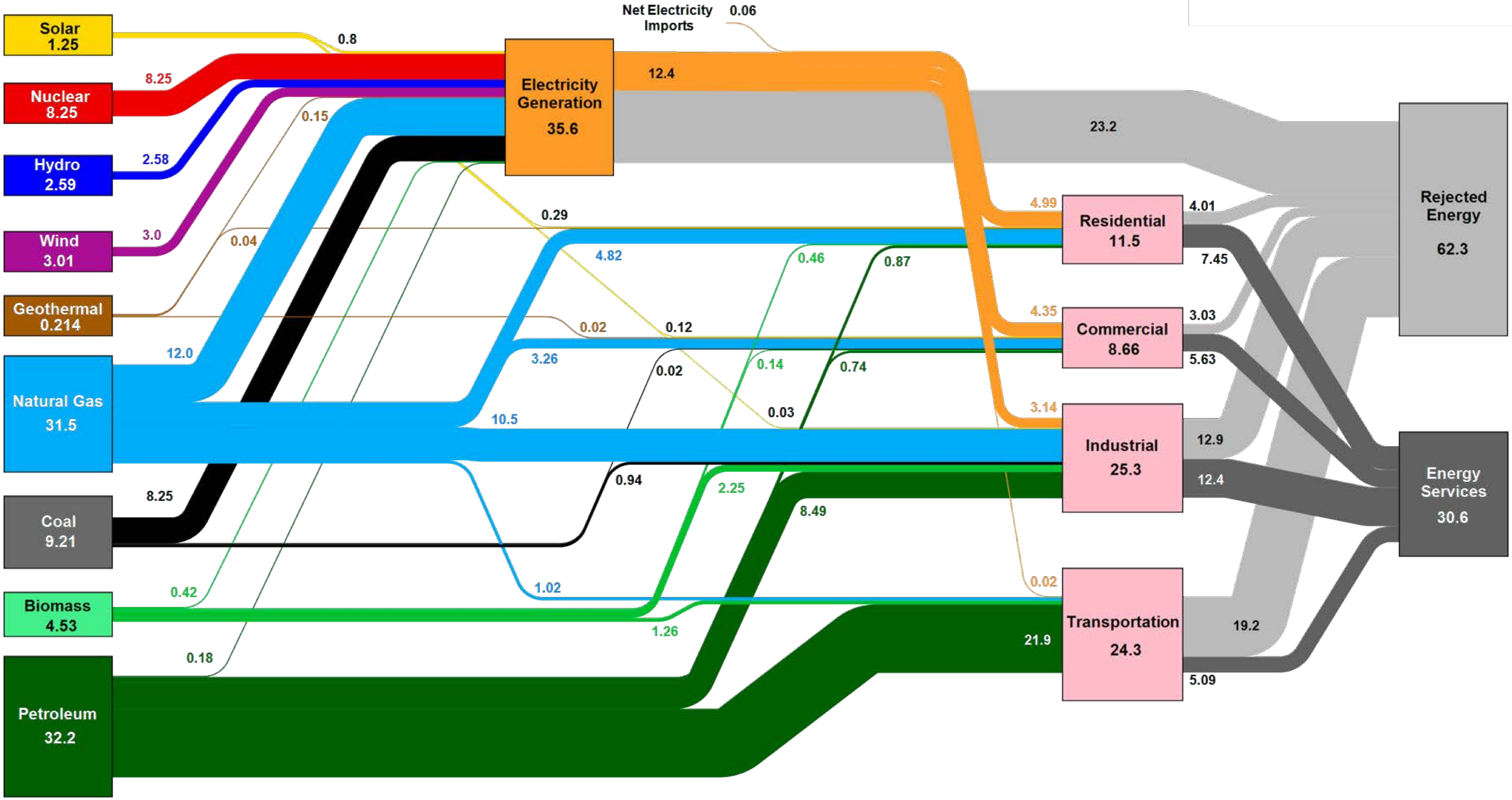
NATIONAL ENERGY TECHNOLOGY LABORATORY

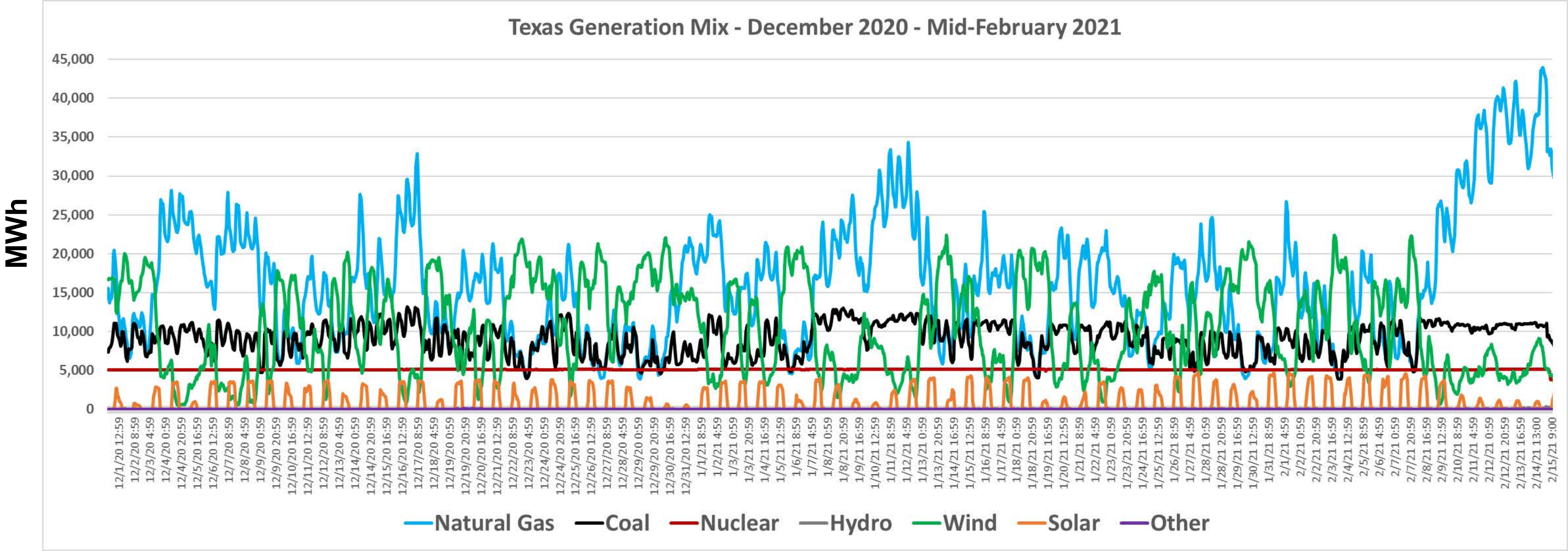
U.S. DEPARTMENT OF ENERGY

Estimated U.S. Energy Consumption in 2020: 92.9 Quads



Source: LLNL March, 2021. Data is based on DOE/EIA MER (2020). 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

Variability in Electricity Production Requires Flexibility



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Decarbonizing & Expanding the U.S. Industrial Sector

Shell Cracker Nears 'Peak Construction'

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Process Intensification & Modularization

- **Intensification** smaller, cleaner, and more energy-efficient technology
  - Reactive distillation
  - Dividing wall columns
  - Rotating packed bed
  - Microreactors
- **Modular design**
  - *“Numbering up” instead of scaling up*
  - Reduced investment risk
  - Improved time to market
  - Increased flexibility
  - Improved safety
  - Reduced on-site construction

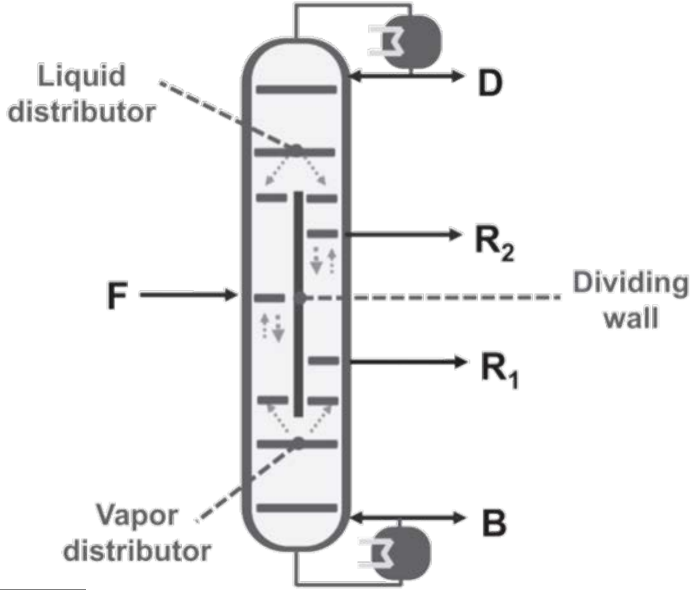
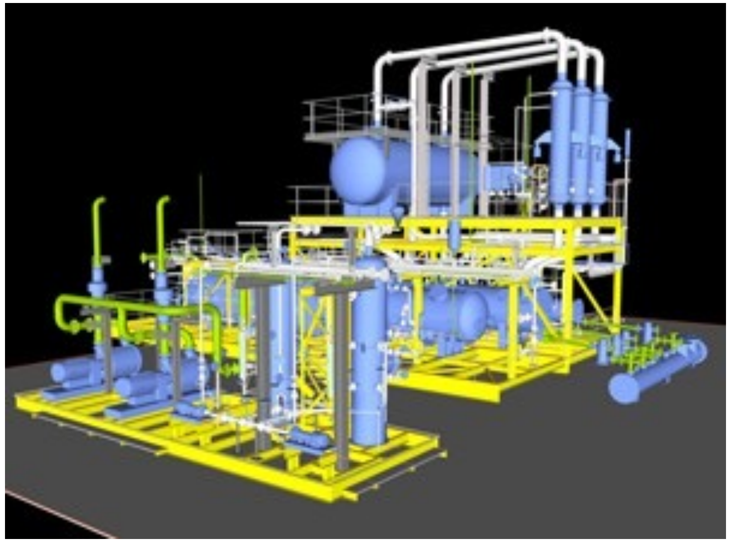
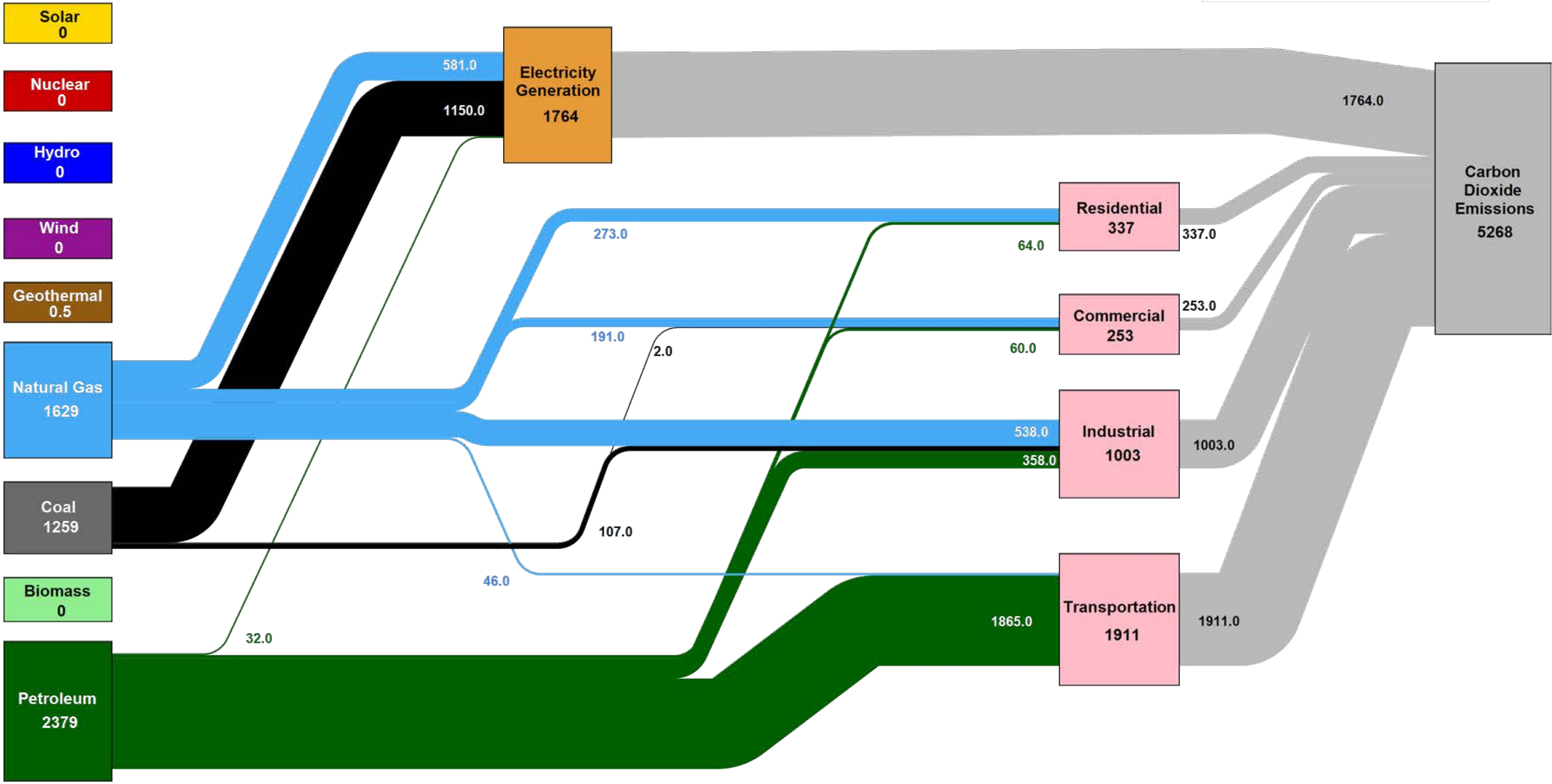


Figure from Rawlings et al., 2019



Estimated U.S. Carbon Dioxide Emissions in 2018: ~5,268 Million Metric Tons



Source: LLNL July, 2019. Data is based on DOE/EIA MER (2018). 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. Carbon emissions are attributed to their physical source, and are not allocated to end use for electricity consumption in the residental, commercial, industrial and transportation sectors. Petroleum consumption in the electric power sector includes the non-renewable portion of municipal solid waste. Combustion of biologically derived fuels is assumed to have zero net carbon emissions – the lifecycle emissions associated with producing biofuels are included in commercial and industrial emissions. Totals may not equal sum of components due to indepedent rounding errors. LLNL-MI-410527

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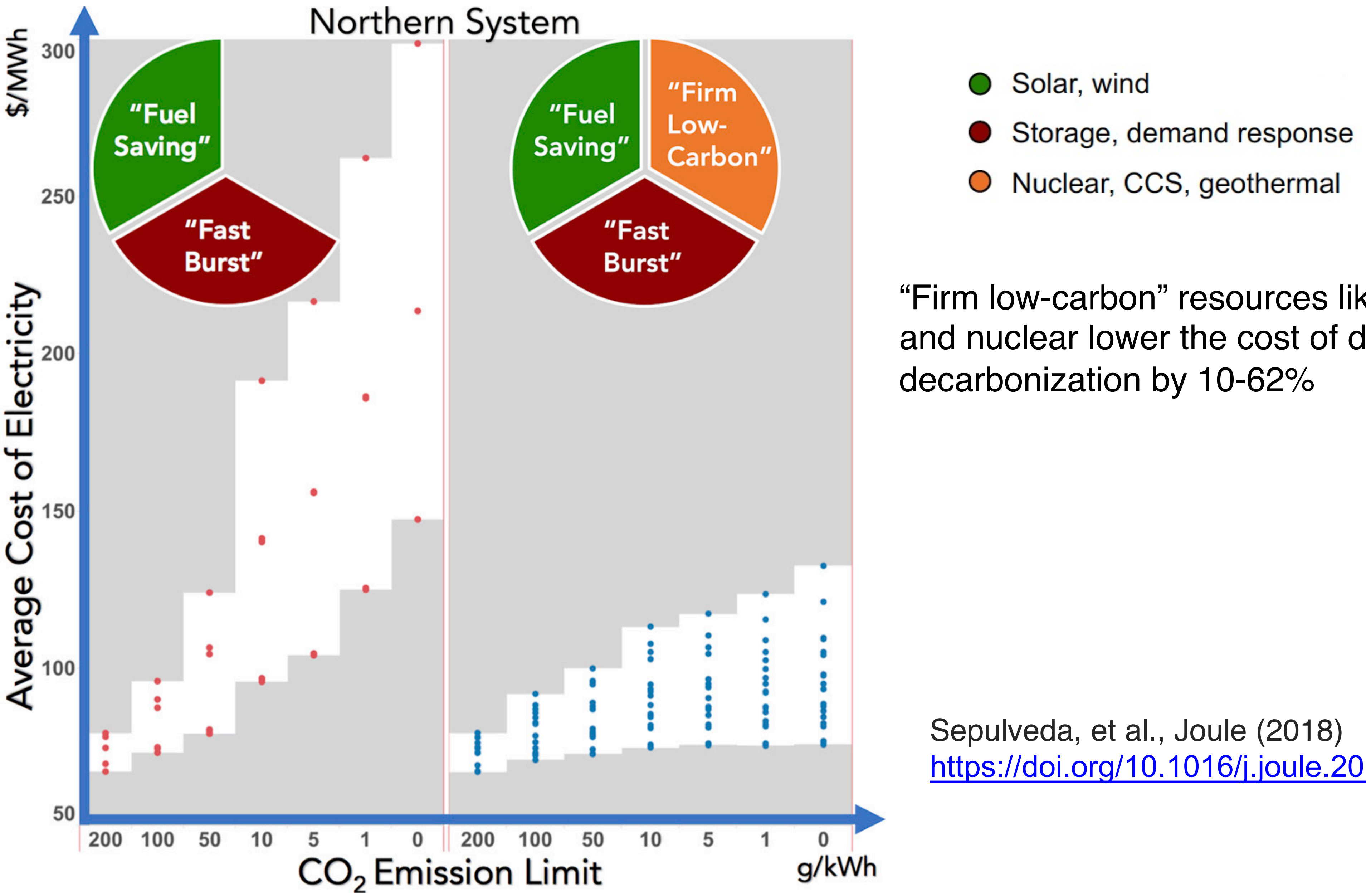
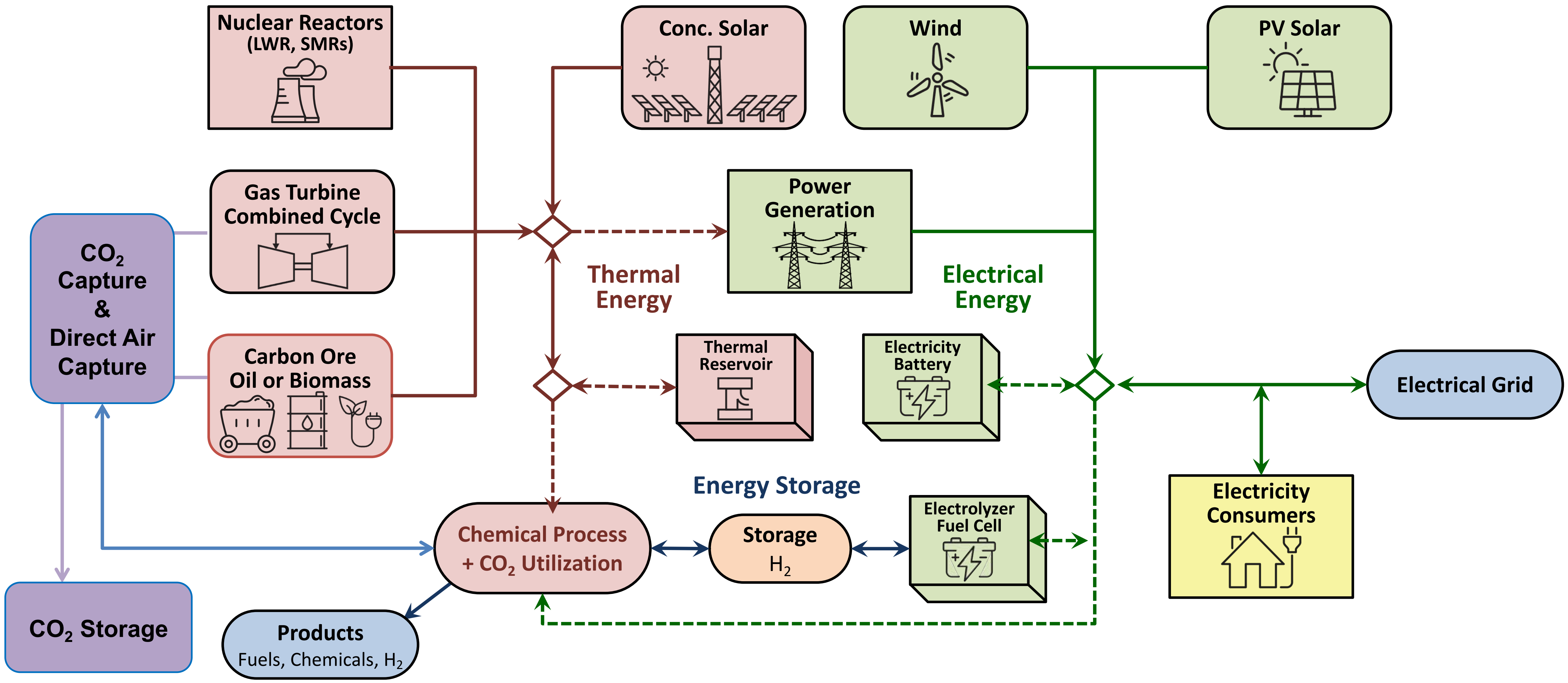
Need for Dispatchable Power for Economic Deep Decarbonization



"Firm low-carbon" resources like CCS and nuclear lower the cost of deep decarbonization by 10-62%

Sepulveda, et al., Joule (2018)
https://doi.org/10.1016/j.joule.2018.08.006

Increasingly Integrated Energy & Process Systems



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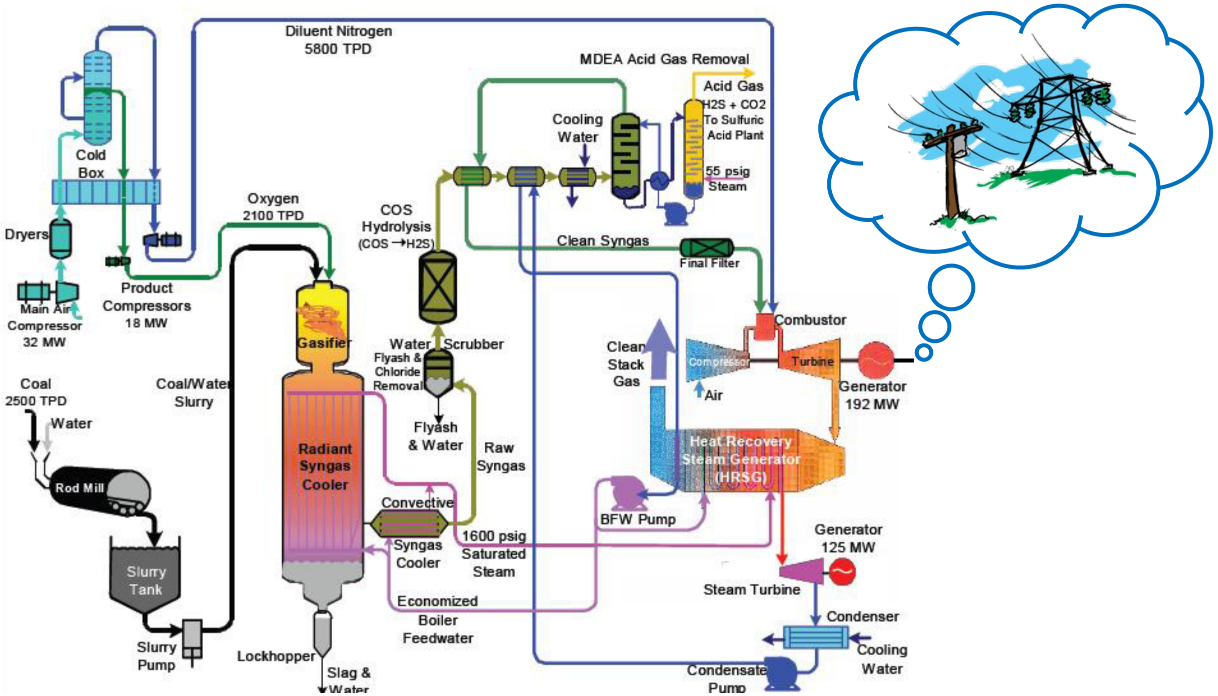
Energy System Analysis is Often Applied in Isolation

Process-centric Modeling

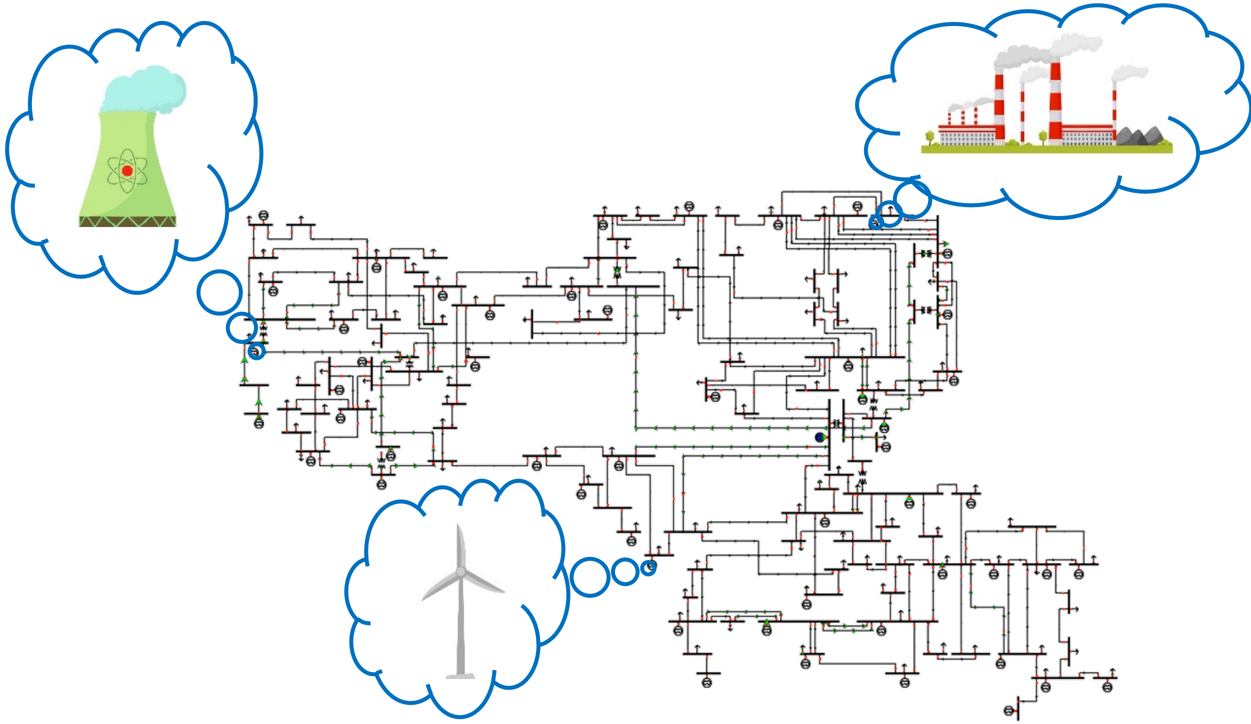
Detailed steady state or dynamic process models, with the grid modeled as an infinite capacity bus



https://www.netl.doe.gov/research/coal/energy-systems/gasification/gasifipedia/igcc-config

Grid-centric Modeling

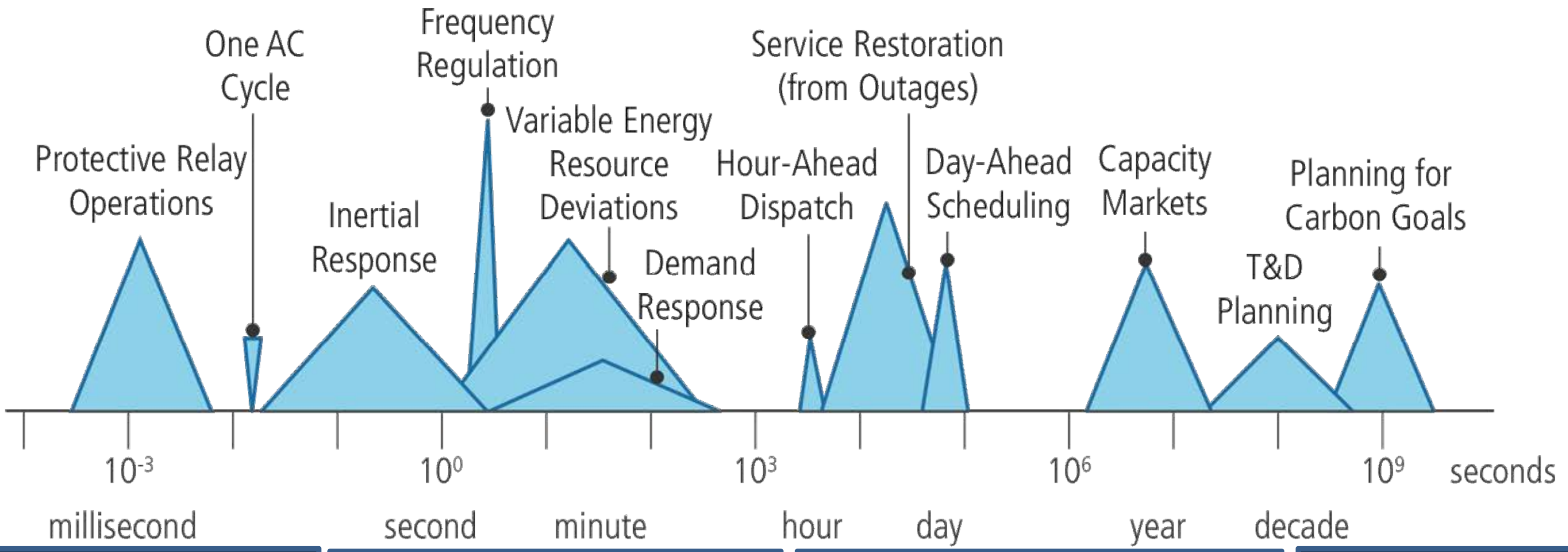
Detailed power flow models,
with individual generators modeled as either
dispatchable point sources or stochastic "negative loads"



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

From Dowling et al. (2020)

Multiple Time Scales & Perspectives Across Tools



Real-Time Operations	Electricity Grid Dispatch, Power Flow	Capacity Expansion 20-30 Year Horizon	Energy Economy Models
High frequency dynamics	Complex effects of new generators	Difficult to value flexibility, reliability	Long time horizons Macro-economics

Process/Generator – Integrated Energy Systems
Design, Operation/Control, Dynamics, Multiple Products

Multi-Sectoral Interactions & Infrastructure
Natural Gas & Fuels, Transportation, Heat, Hydrogen, Chemicals, Other

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

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

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

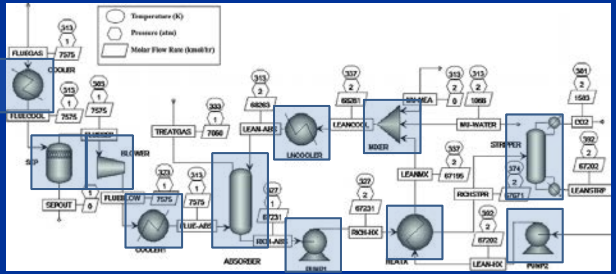
Optimization over
degrees of freedom only

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

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]

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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.

IDAES Integrated Platform

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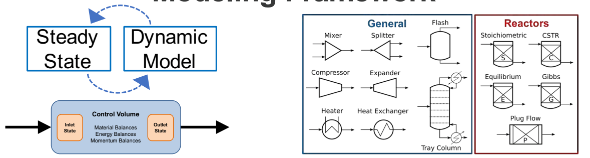
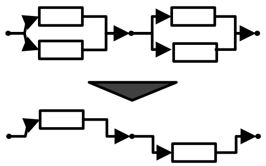
Modeling Framework



Hierarchical - Steady-State & Dynamic - Model Libraries

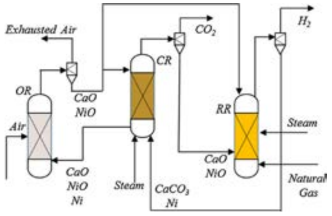
Conceptual Design	Plant Design Process Optimization	Process Operations Dynamics & Control	Uncertainty Quantification Robust Optimization	AI/ML Surrogate Modeling	Enterprise Optimization Grid & Planning	Materials Optimization

Conceptual Design



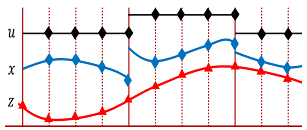
PYOMO GDP

Plant Design Process Optimization

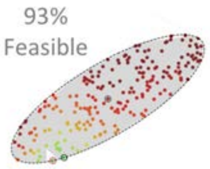


Process Operations Dynamics & Control

caprese



Uncertainty Quantification Robust Optimization

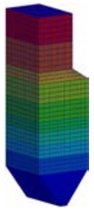


PyROS

AI/ML Surrogate Modeling

ALAMO

PySMO



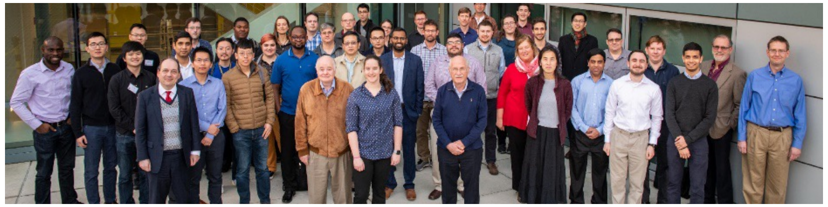
Enterprise Optimization Grid & Planning

Materials Optimization

MatOpt Nanomaterials optimization

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

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



2020 R&D 100 WINNER

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

Examples of IDAES Optimization Approach

- Process/Grid Coupling
  - Understanding complex interactions across scales
- Carbon Capture System Design
  - Technical Risk Reduction through UQ and Robust Optimization
  - Incorporating flexible operations in design decisions
- Integrated Energy System Design
  - Multi-input, multi-output dynamic energy systems
- Expansion Planning
  - Achieving decarbonization goals while maintaining reliability

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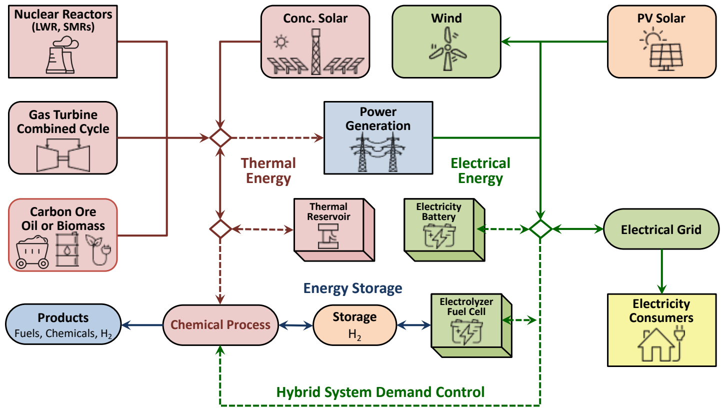
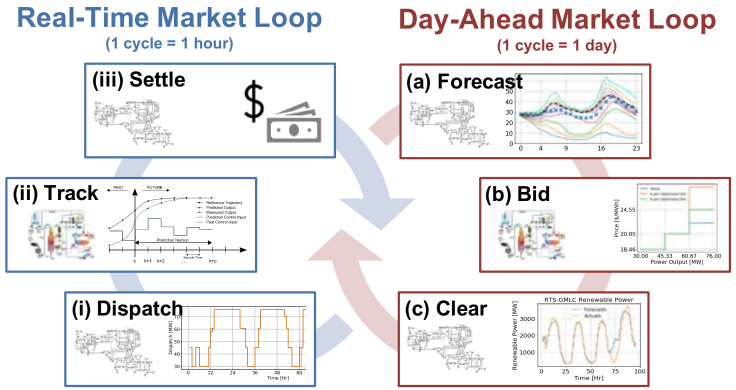
Bridging Timescales Enables Unique Analyses & Design of IES

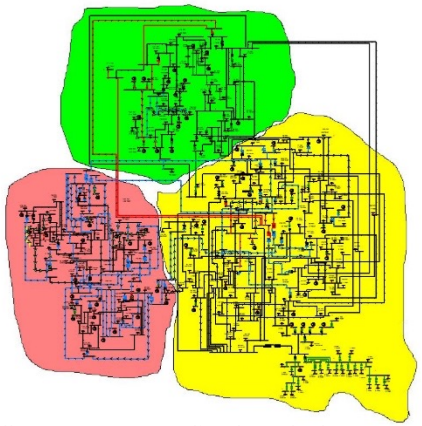
High-Fidelity Process Modeling



Integrated Resource-Grid Model



Grid Modeling



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

1. Elucidate complex relationships between resource dynamics and market dispatch (with uncertainty, beyond price-taker assumption)
2. Predict the economic opportunities and market impacts of emerging technologies (tightly-coupled hybrid energy systems)
3. Guide conceptual design & retrofit to meet current and future power grid needs

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

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.

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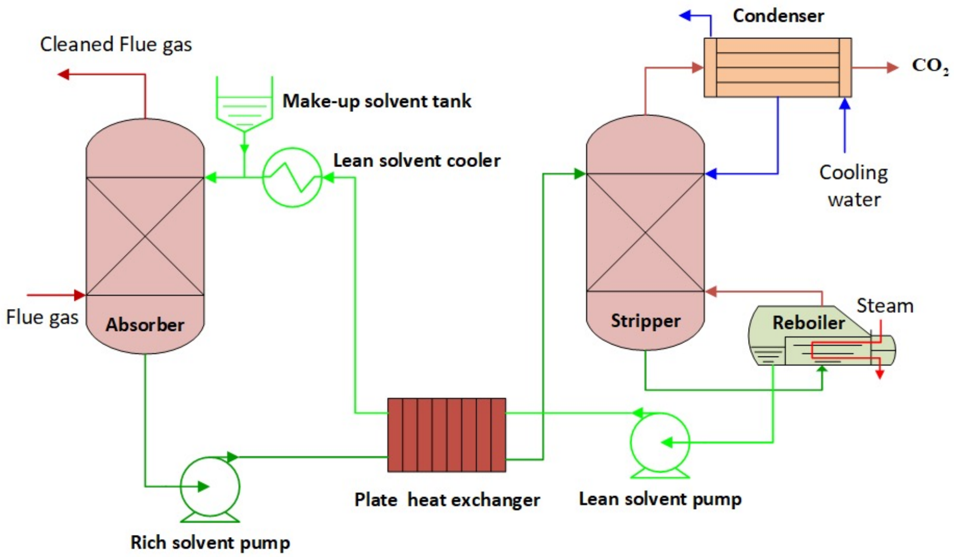
Predictive Process Modeling and Optimization

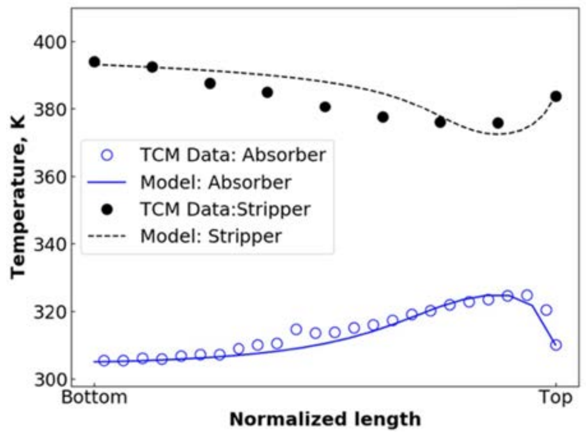
Identifying optimal operational strategies and process designs

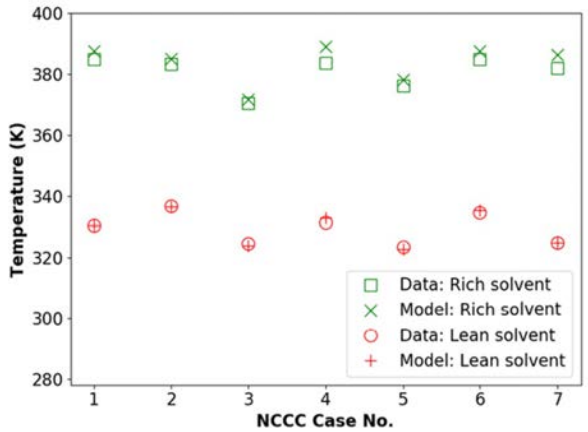


- Modular, multi-scale, dynamic rate-based
- Film model
  - Multi-component mass & heat transport
  - Simultaneous reaction & transport of molecular & ionic species
- Rigorous properties
  - Modified eNRTL model for mixed solvent systems

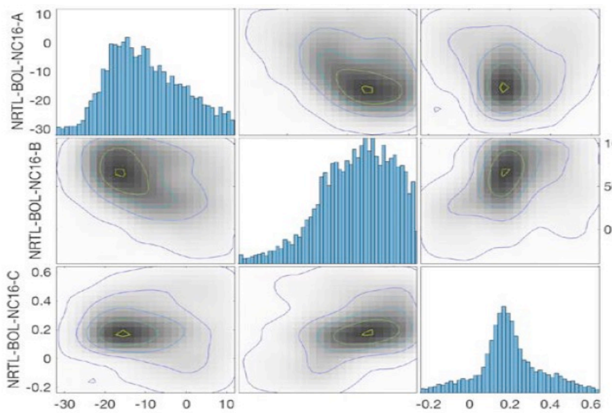
[Akula, et. al., 2021, I&EC Research, 60(14), 5176-5193]()

Model Validation

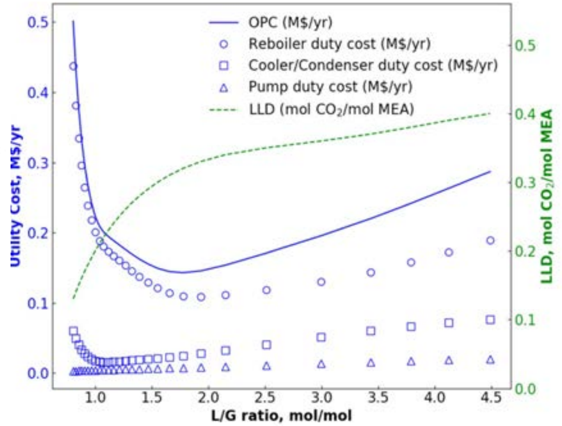




Parameter Estimation and Uncertainty Quantification



Process Optimization



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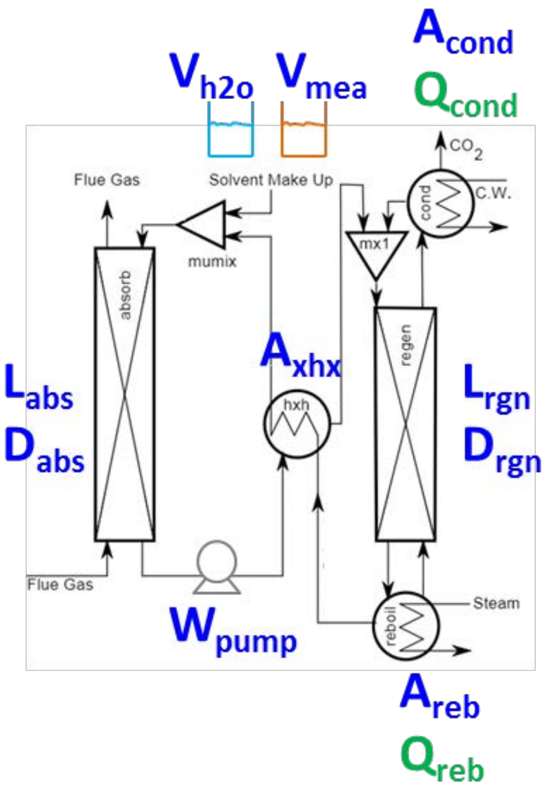
Robust Design to Reduce Technical Risk

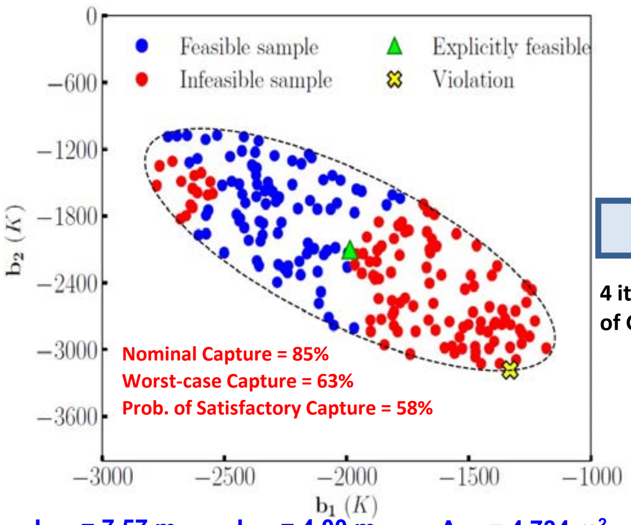
Inherent uncertainty in process design models

Operational uncertainty: e.g., fluctuations in feed
Economic uncertainty: e.g., cost of utilities
Epistemic uncertainty: e.g., mass/heat transfer, kinetics



Deterministic Solution

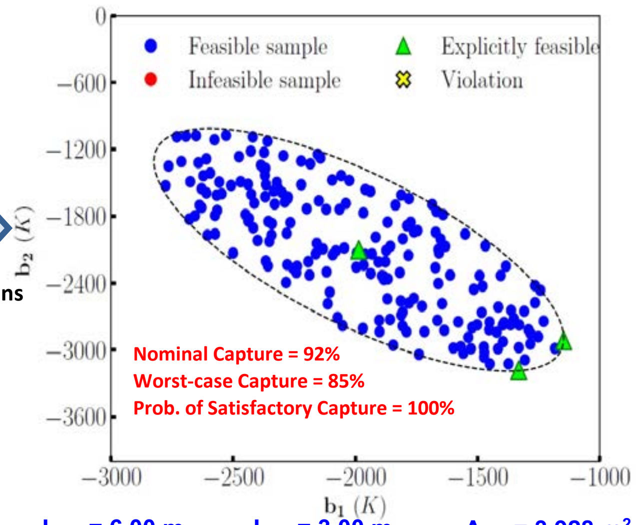
Cost: \$7.25 MM/yr
Second-stage Cost: \$5.19 MM/yr



4 iterations of GRCS

Robust Solution

Cost: \$10.90 MM/yr
Expected Second-stage Cost: \$5.51 MM/yr



Deterministic: L_{abs} = 7.57 m, D_{abs} = 4.95 m; L_{reg} = 4.00 m, D_{reg} = 3.44 m; A_{xhx} = 4,734 m^2, Q_{reb} = 18 MW, Q_{con} = -4.5 MW

Robust: L_{abs} = 6.00 m, D_{abs} = 4.96 m; L_{reg} = 3.00 m, D_{reg} = 4.04 m; A_{xhx} = 3,928 m^2, Q_{reb} = [17.6, 20.5] MW, Q_{con} = [-6.7, -0.53] MW

Deteministic design
fails to meet CO_2 capture performance requirement with a 33% probability

Robust design
guarantees CO_2 capture in all scenarios; cost increase is kept to the minimum necessary to achieve this

Robustness achieved
utilizes smaller equipment overall, putting more emphasis on reboiler and condenser duty control

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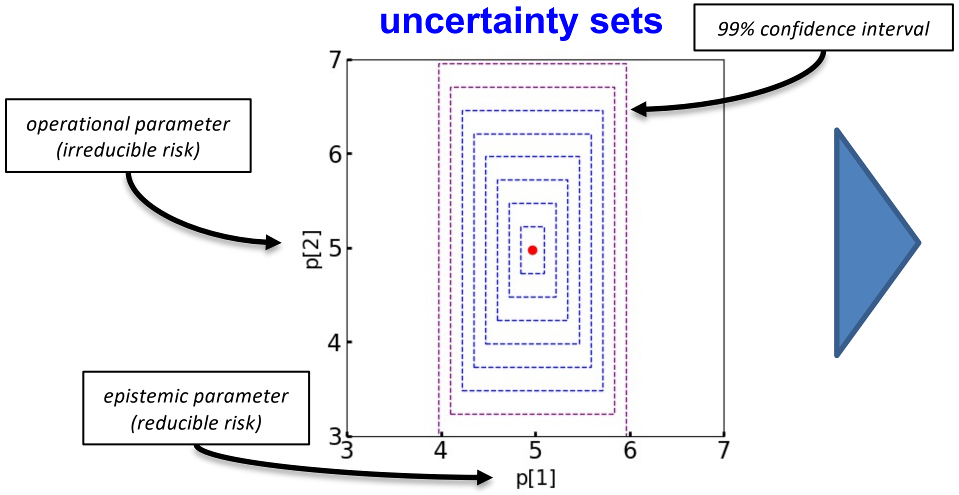
N.M. Isenberg, P. Akula, J.C. Eslick, D. Bhattacharyya, D.C. Miller and C.E. Gounaris (2021). A Generalized Cutting-Set Approach for Nonlinear Robust Optimization in Process Systems Engineering Applications. *AIChE Journal*, 67(5):e17175, *DOI 10.1002/aic.17175*

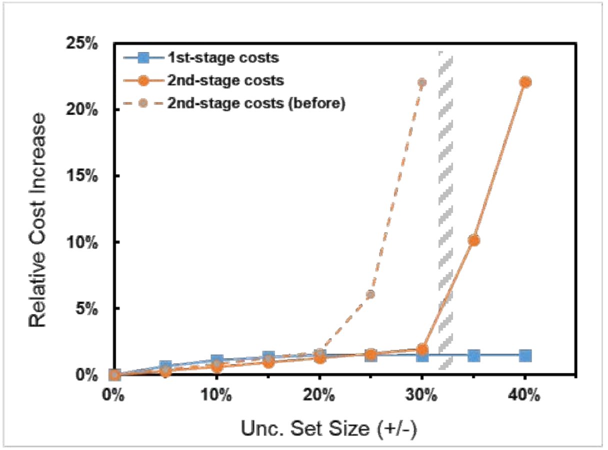
Reducing the Price of Robustness

- The PoR provides an **upper limit on the $ worth spending** to reduce parameter uncertainty
  - e.g., do more "science" to improve our property models
- Factors to consider when deciding whether to go back to the drawing board:
  - plausibility of reducing uncertainty (e.g., epistemic uncertainty)
  - the cost of conducting additional research to improve uncertainty confidence
  - the time it will take to do so (cost of delaying the investment)
  - the anticipated improvement in the risk-reward trade-off
- Quantifying the improvement:

Hierarchy of uncertainty sets



Evolution of costs for increasingly robust designs



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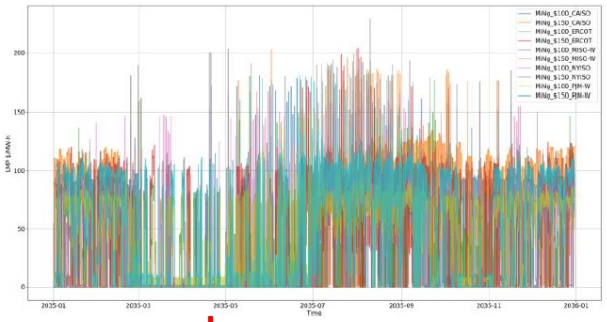
Multi-scale Surrogate Modeling

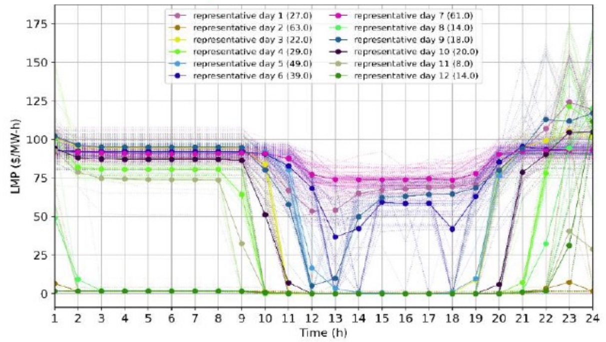
Linking models across length/time-scales with minimal loss of accuracy

Process LMP Signals

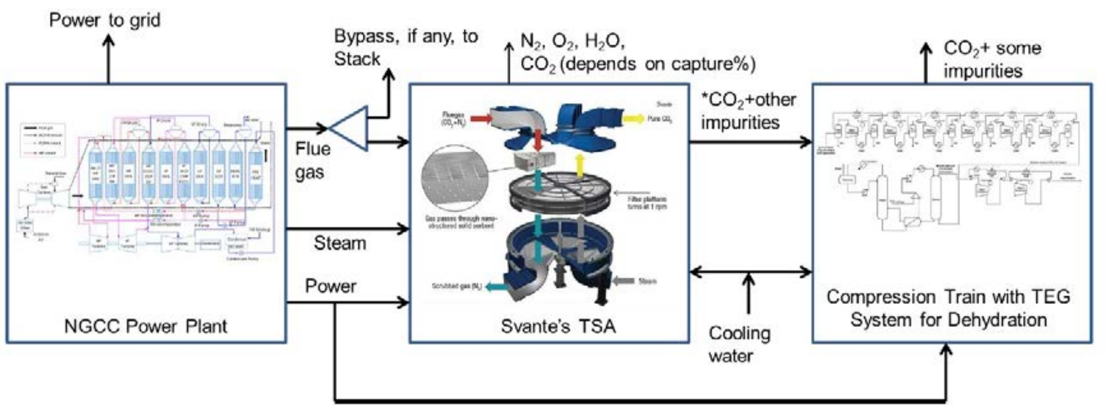
Input from ARPA – E
- Locational Marginal Price (LMP) signal (in \$/MWh)



Identify representative days

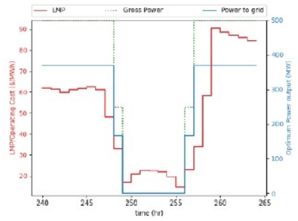


Develop Rigorous and Reduced-order (surrogate) Process Models



Formulate and Solve Multi-period Optimization Problem

Result: Optimal solution maximizing the Net Present Value (NPV)
- Optimal design of the capture system
- Optimal power schedule
- Detailed cash flows



Should capture system be built? (i.e., Is it cheaper to pay a carbon tax?)

If yes, what is the optimal size and capture rate?

How do various potential market scenarios impact results?

Gooty, et al., 2022, in preparation

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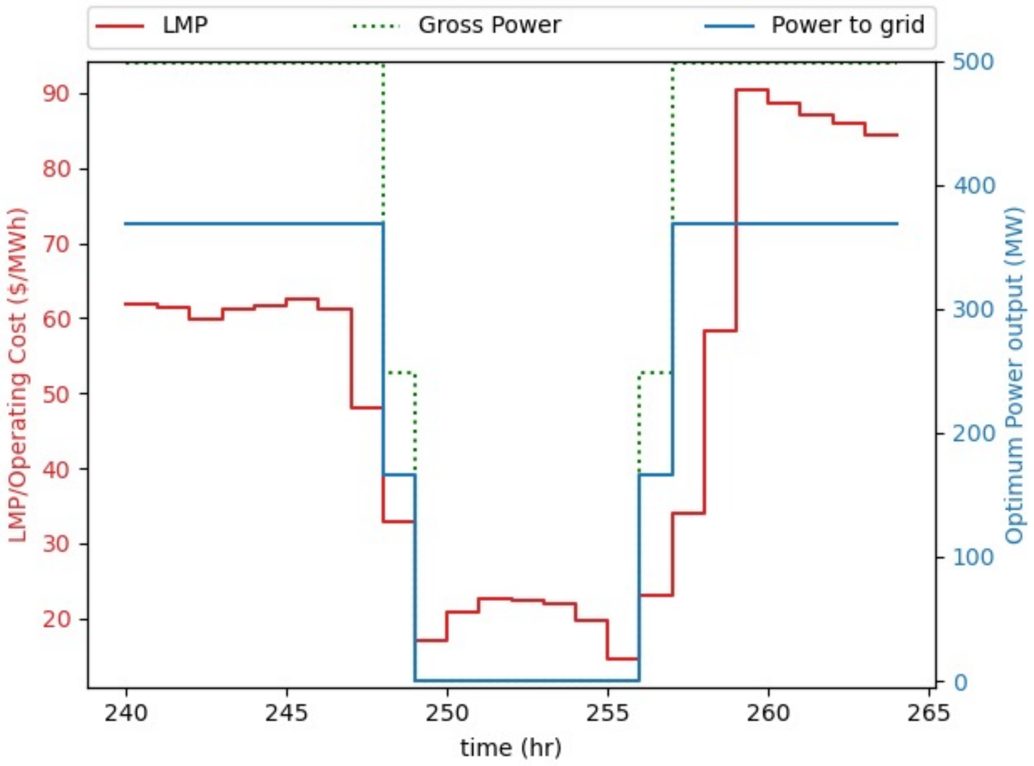
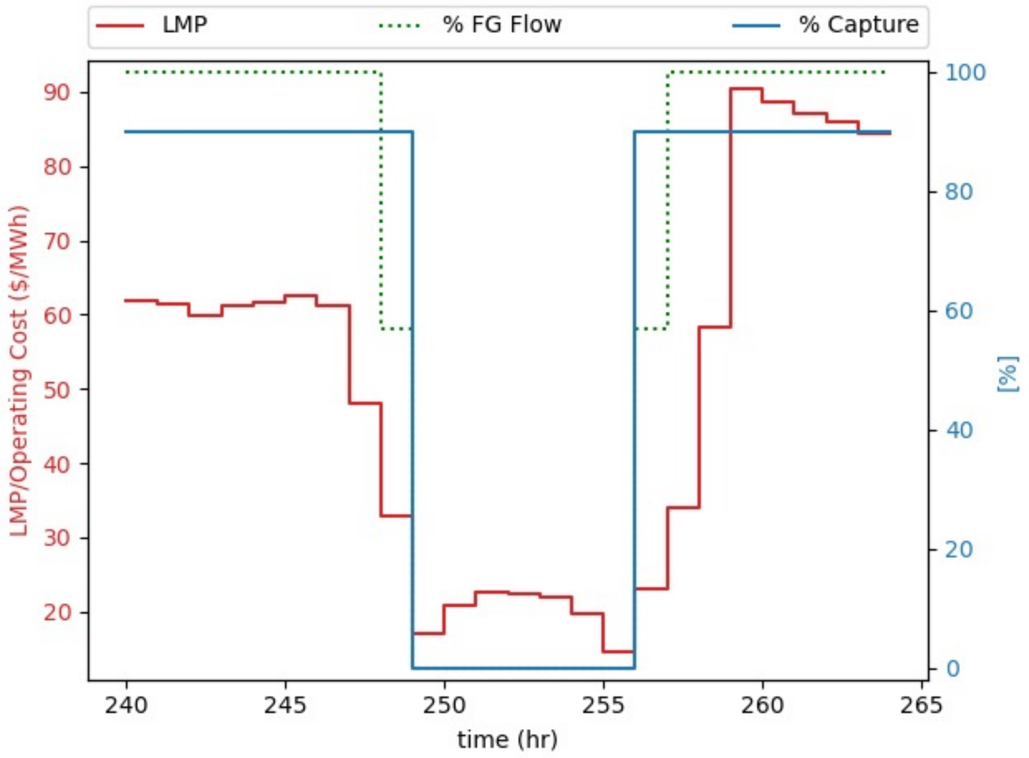
Flexible Operations Scenario with Carbon Capture



Optimal Power Schedule



Optimal Operation of the Capture System

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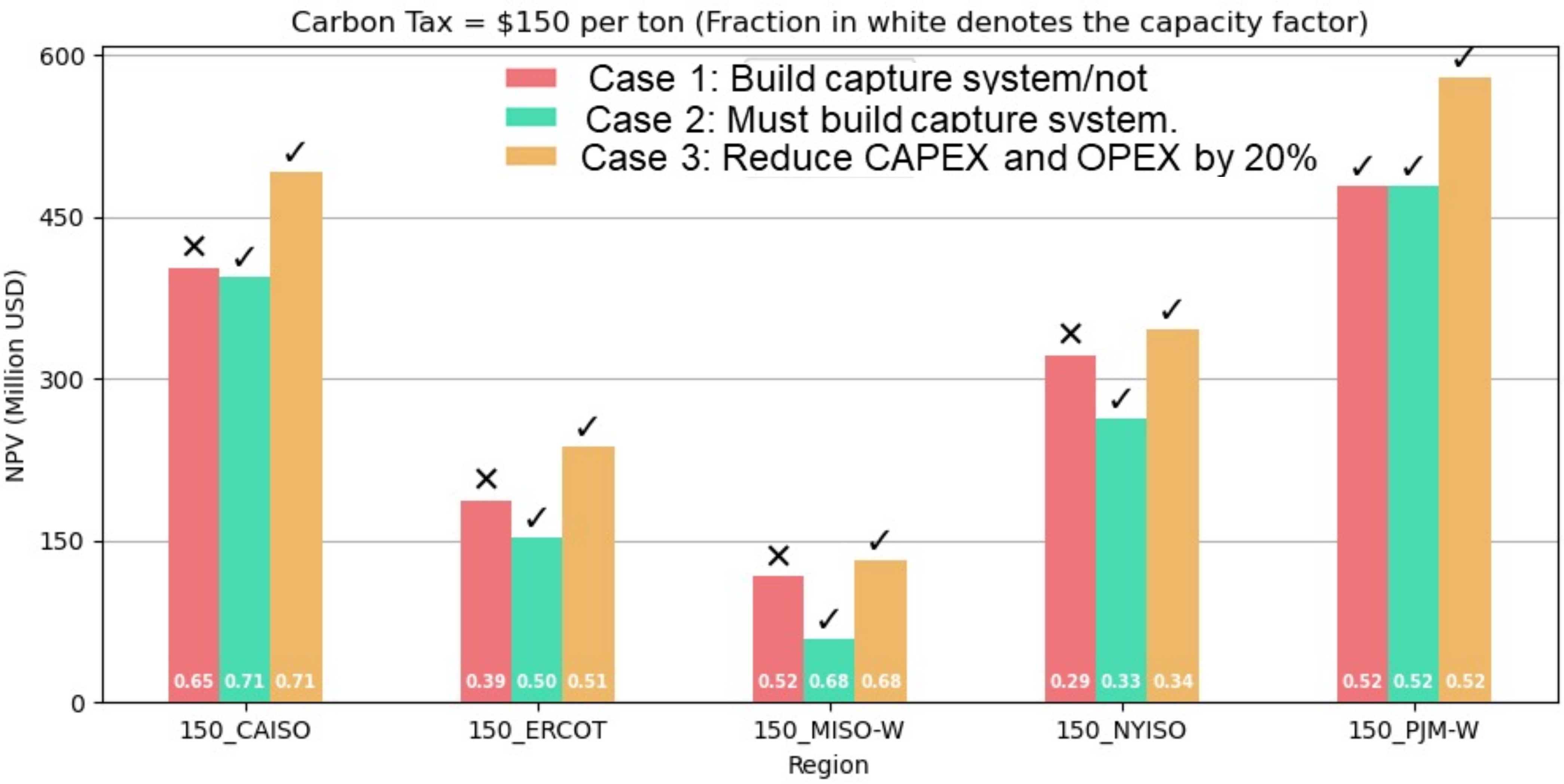
Example Scenarios: Flexible Capture NPV Optimization



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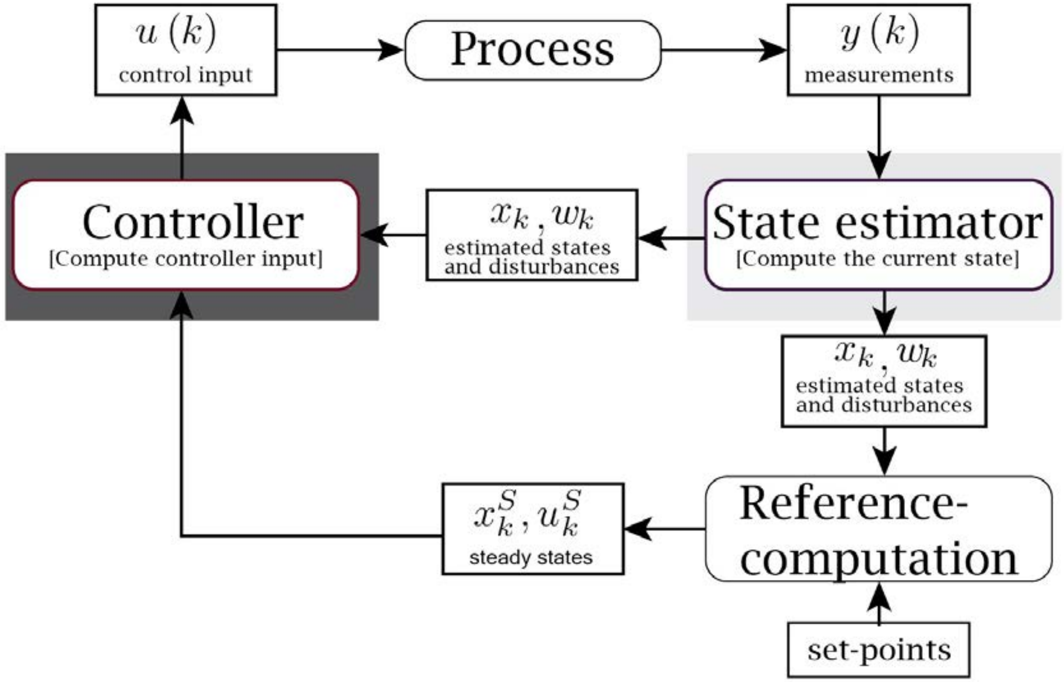
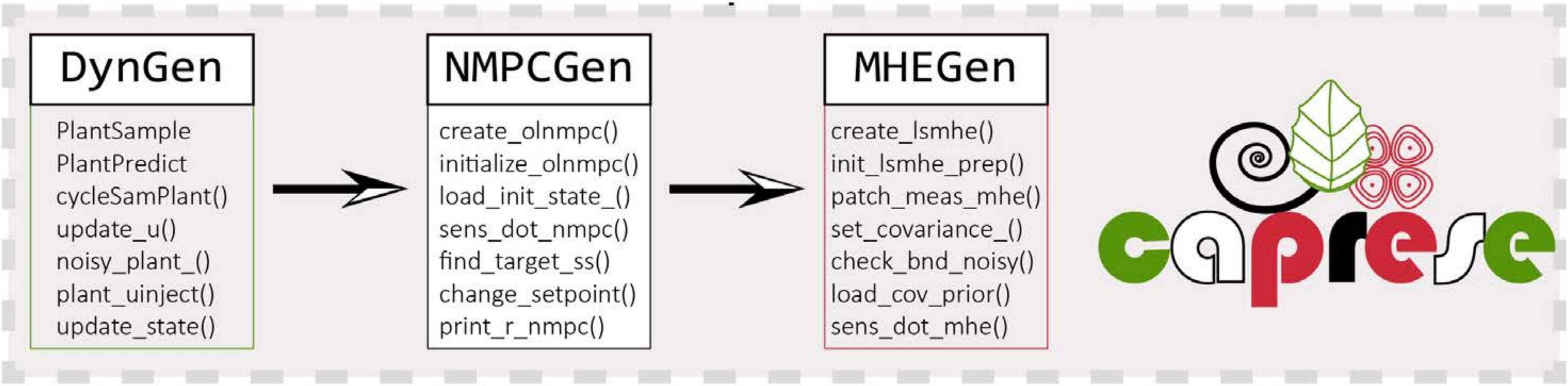
CAPRESE: Control and Adaptation w PREdictive SEnsitivity)





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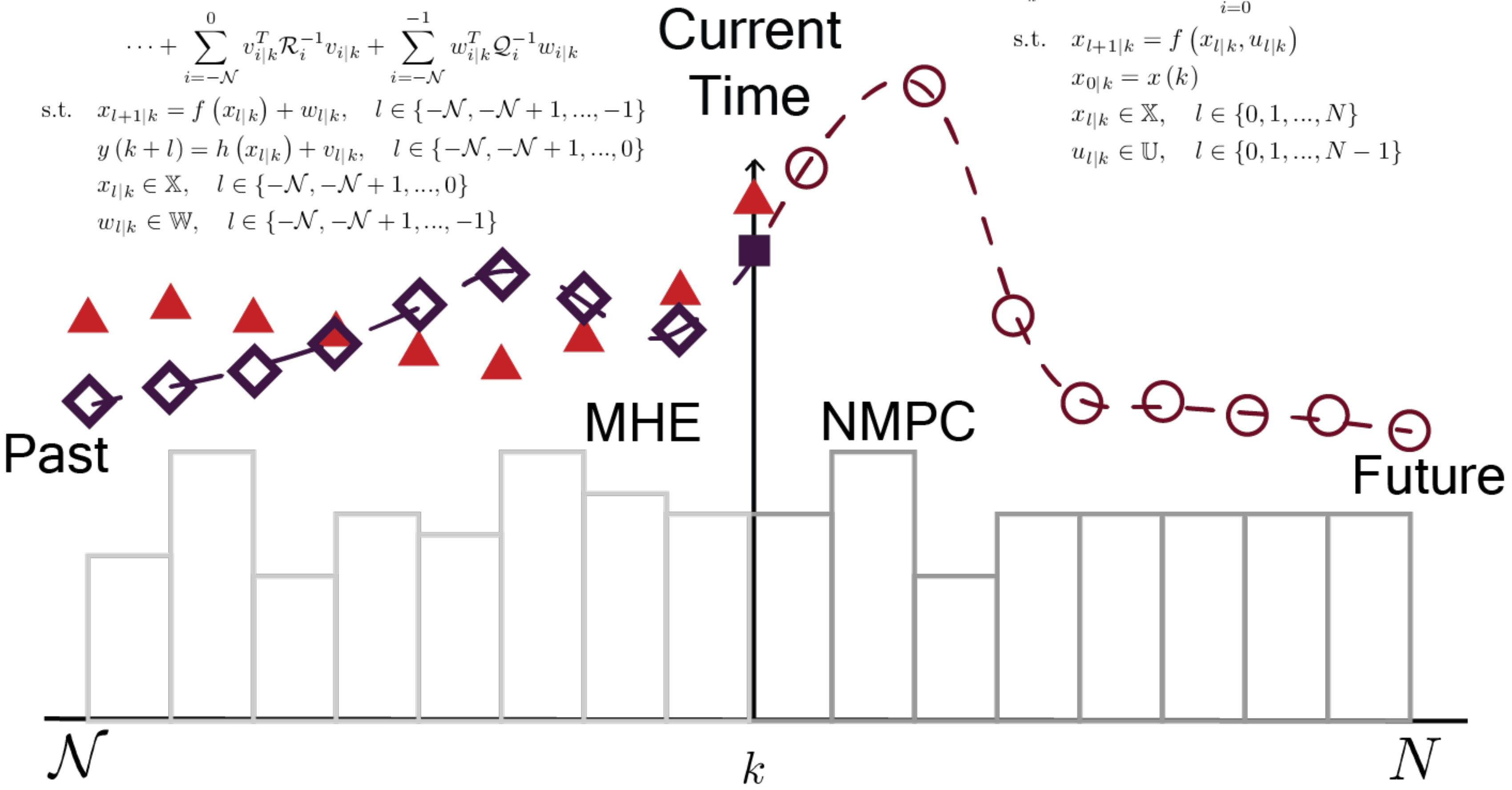
Model-based Estimation and Control: MHE and NMPC

$$\mathcal{M}\left(\Pi_{-\mathcal{N}|k-1}, \hat{x}_{-\mathcal{N}|k-1}, y(k), \ldots, y(k-\mathcal{N})\right):$$

$$\begin{aligned} \min_{x_{-\mathcal{N}}, \boldsymbol{w}_k} \quad & \Phi_{-\mathcal{N}}\left(x_{-\mathcal{N}|k}, \hat{x}_{-\mathcal{N}|k-1}, \Pi_{-\mathcal{N}|k-1}\right) + \cdots \\ & \cdots + \sum_{i=-\mathcal{N}}^{0} v_{i|k}^T \mathcal{R}_i^{-1} v_{i|k} + \sum_{i=-\mathcal{N}}^{-1} w_{i|k}^T \mathcal{Q}_i^{-1} w_{i|k} \\ \text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}\right) + w_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, -1\} \\ & y(k+l) = h\left(x_{l|k}\right) + v_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, 0\} \\ & x_{l|k} \in \mathbb{X}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, 0\} \\ & w_{l|k} \in \mathbb{W}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, \ldots, -1\} \end{aligned}$$

$$\mathcal{P}\left(x(k)\right):$$

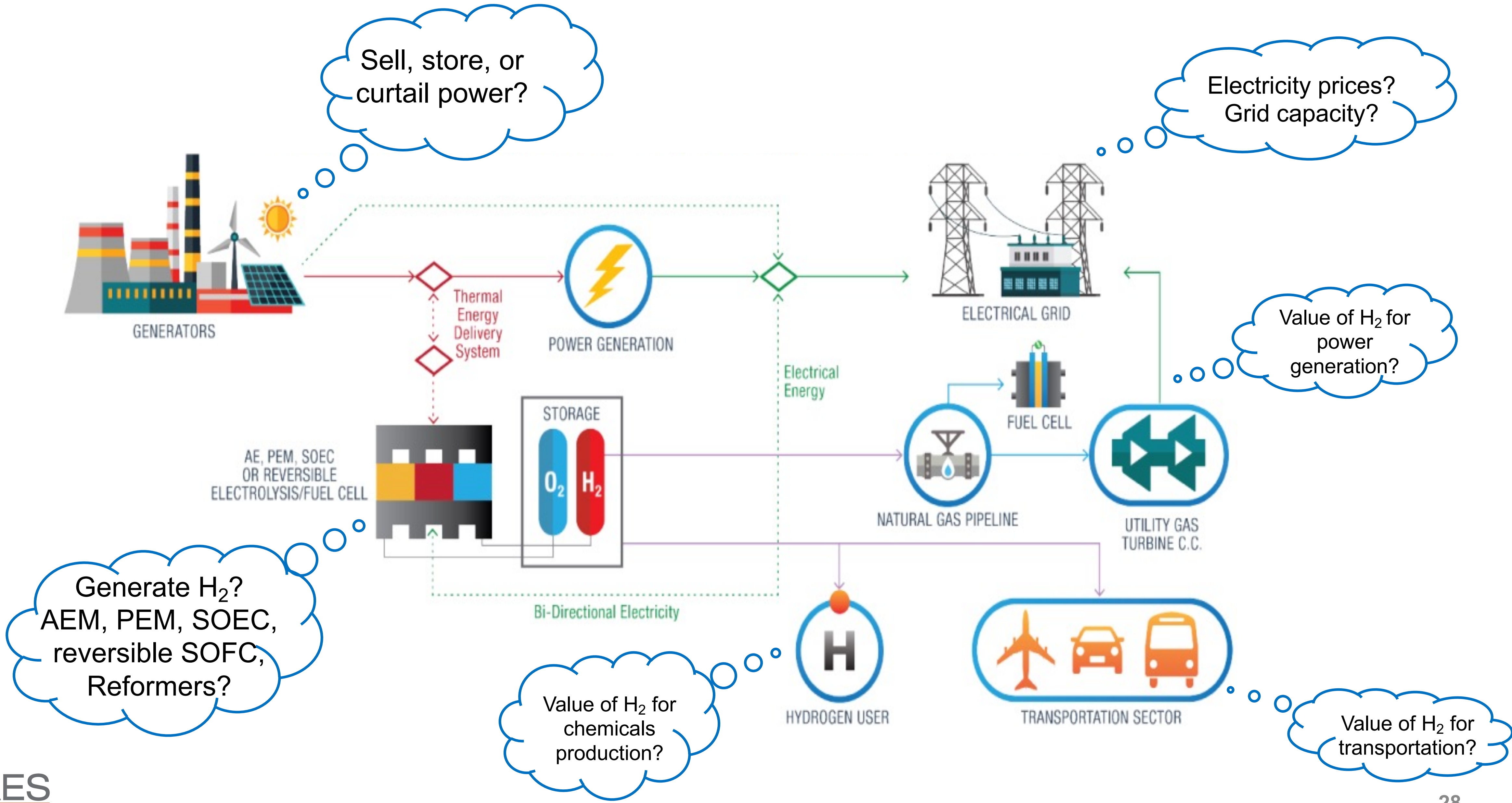
$$\begin{aligned} \min_{\boldsymbol{u}_k} \quad & \varphi_N\left(x_{N|k}\right) + \sum_{i=0}^{N-1}\left[x_{i|k}^T Q x_{i|k} + u_{i|k}^T R u_{i|k}\right] \\ \text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}, u_{l|k}\right) \\ & x_{0|k} = x(k) \\ & x_{l|k} \in \mathbb{X}, \quad l \in \{0, 1, \ldots, N\} \\ & u_{l|k} \in \mathbb{U}, \quad l \in \{0, 1, \ldots, N-1\} \end{aligned}$$



Examples of IDAES Optimization Approach

- Process/Grid Coupling
  - Understanding complex interactions across scales
- Carbon Capture System Design
  - Technical Risk Reduction through UQ and Robust Optimization
  - Incorporating flexible operations in design decisions
- **Integrated Energy System Design**
  - **Multi-input, multi-output dynamic energy systems**
- Expansion Planning
  - Achieving decarbonization goals while maintaining reliability

Integrated Energy System For Power and H_2 Production



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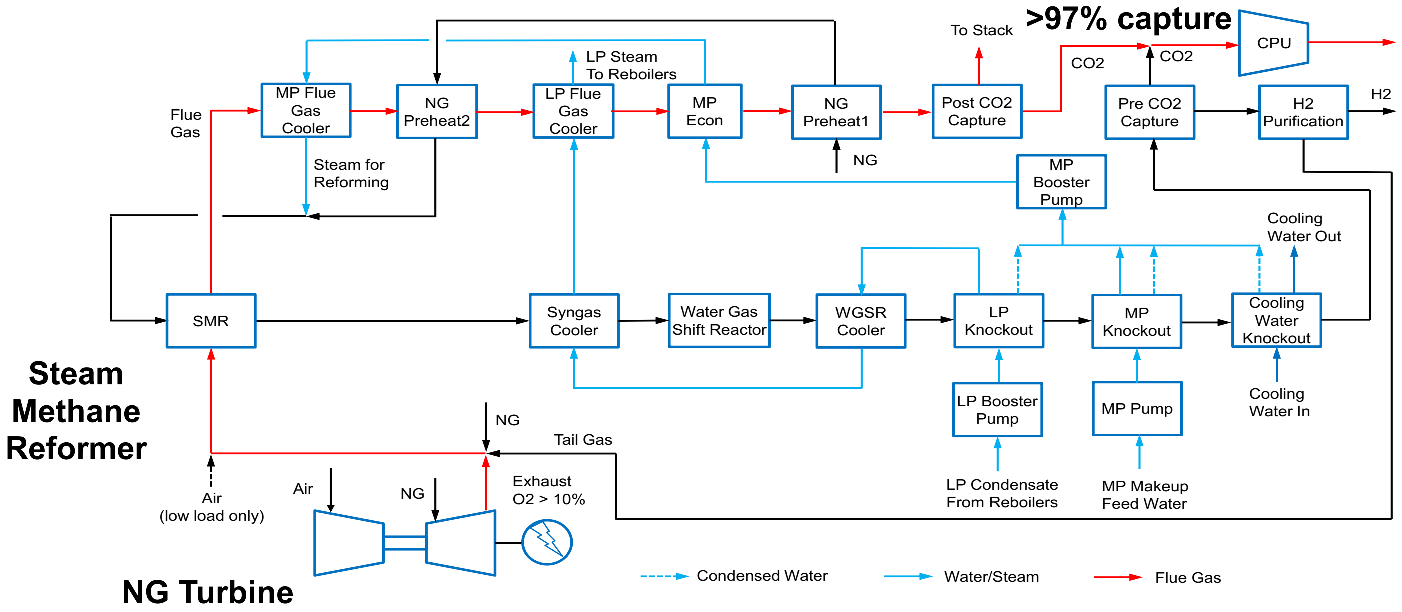
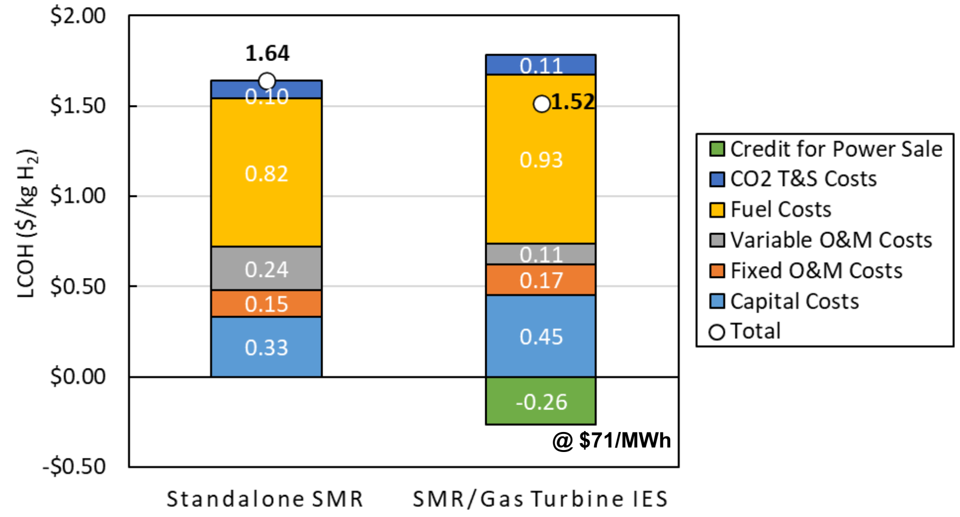
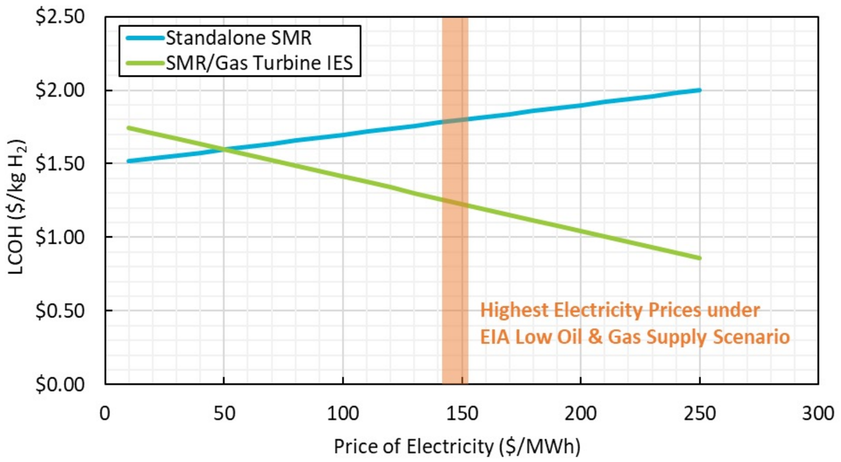
Optimization of Integrated Energy Systems

Reforming-based Systems for Low Carbon Power and Hydrogen





- Integrating gas turbine with SMR improves thermal efficiency
- Shared carbon capture system for power and H_2.
- Significantly reduces cost of low carbon H_2 under future energy scenarios
- Marginal cost of low carbon electricity production below $30/MWh
- Highlighted in Hydrogen Energy Earthshot Strategy Vision document



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SOFC/SOEC: Optimization of Integrated Energy Systems

maximize

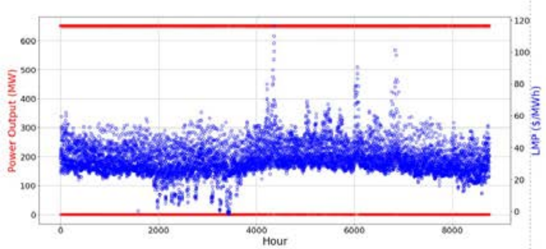
$$\sum_{t \in T} \underbrace{\pi_{p,t} p_t}_{revenue\ from\ power} + \underbrace{\pi_h h_t}_{revenue\ from\ hydrogen} - \underbrace{\left(C_{operating}(p_t, h_t) + C_{capital+fixedO\&M}(P_{max}, H_{max})\right)}_{sum\ of\ costs}$$

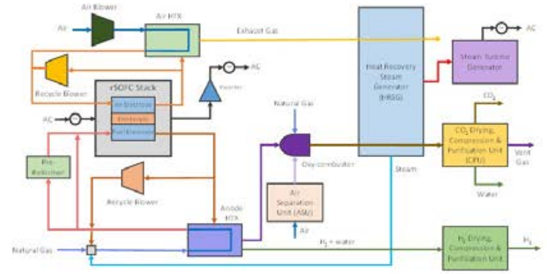
where

t	Minutes or hours over a given time horizon, T
$\pi_{p,t}$	Locational marginal price of electricity at time t
p_t	Power output at time t
π_h	Assumed selling price for H_2
h_t	H_2 production rate at time t
P_{max}	Maximum power output of the plant
H_{max}	Maximum H_2 output of the plant, and
$c_{operating}$ and $c_{capital+fixedO\&M}$	Algebraic surrogate models (i.e., equations) for the variable and fixed costs, respectively.

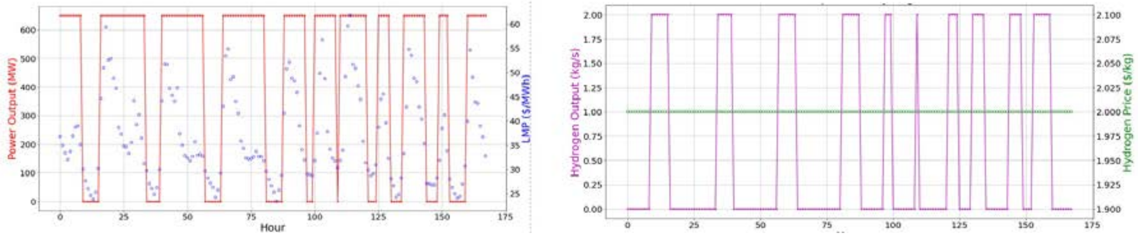
rSOFC + CCS dispatch, 2015 CAISO
Power capacity factor 0.48, H2 capacity factor 0.52

Full year:

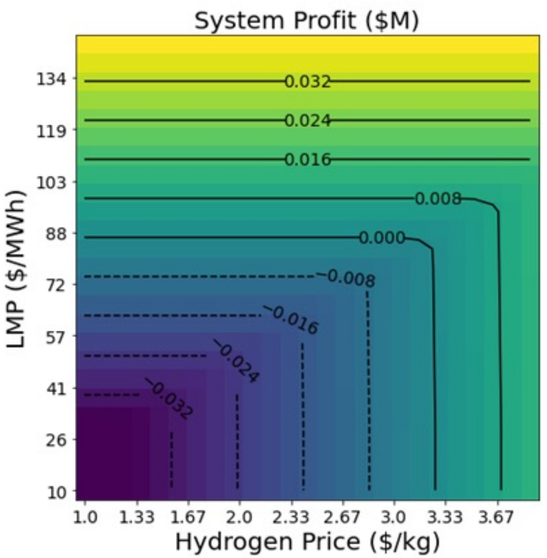




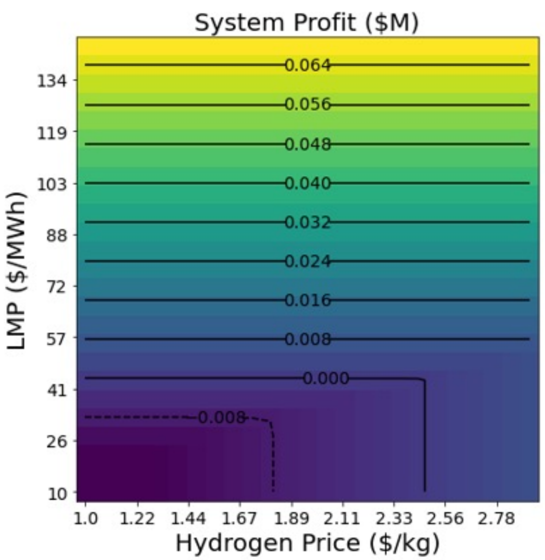
Week 1:



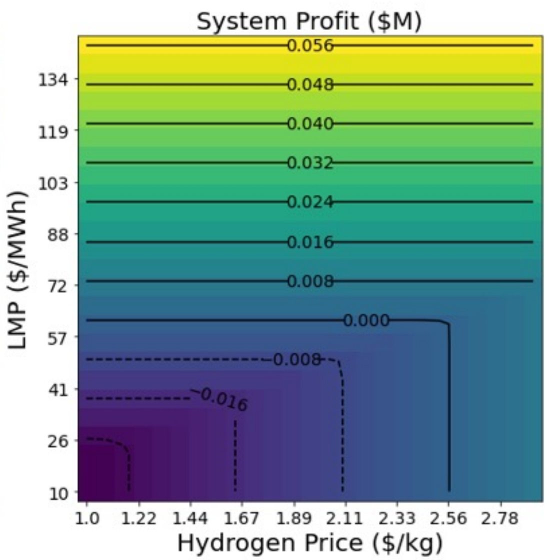
NGCC+SOEC



rSOFC



SOFC+SOEC



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Examples of IDAES Optimization Approach

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  - **Achieving decarbonization goals while maintaining reliability**

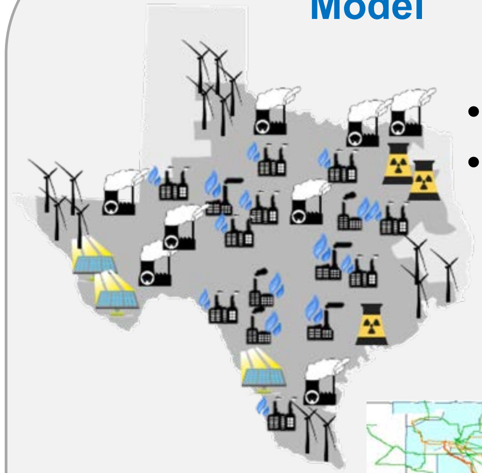
Expansion Planning: Co-optimization of Investment + Operation

INPUT

- **Generation**
  - **Investments** (overnight capital costs, age and lifetime, life extension costs, fuel prices, locations)
  - **Operations** (heat rates, nameplate capacity, reserve capacities, generation limits, ramp rates, emissions, start up fuels/costs, fixed and variable O&M costs, pollutant taxes)
- **Transmission**
  - Overnight costs, lengths, power loss rates, capacities, existing and candidate lines
- **Demand and renewables**
  - Representative profiles, annual load forecasts, available capacity of potential wind and solar sites, wind and solar capacity credits

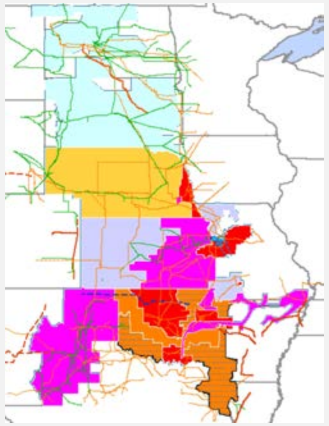
Minimize the **total cost of** operation, investment, and emissions (**net present value**)

Model



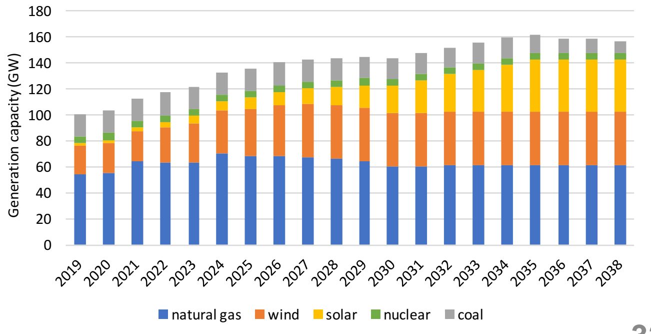
- Generation
- Storage

- Energy sources
  - coal
  - natural gas
  - oil
  - biomass
  - nuclear
  - solar
  - wind



OUTPUT

- **Installments** (generators, transmission lines, storage units)
  - location
  - year
  - type
  - Number and capacity
- **Retirements** (generators, transmission lines, storage units)
  - Year
  - Life extension decision
- **Operation decisions**
  - Approximate power flows
  - Approximate generation schedules



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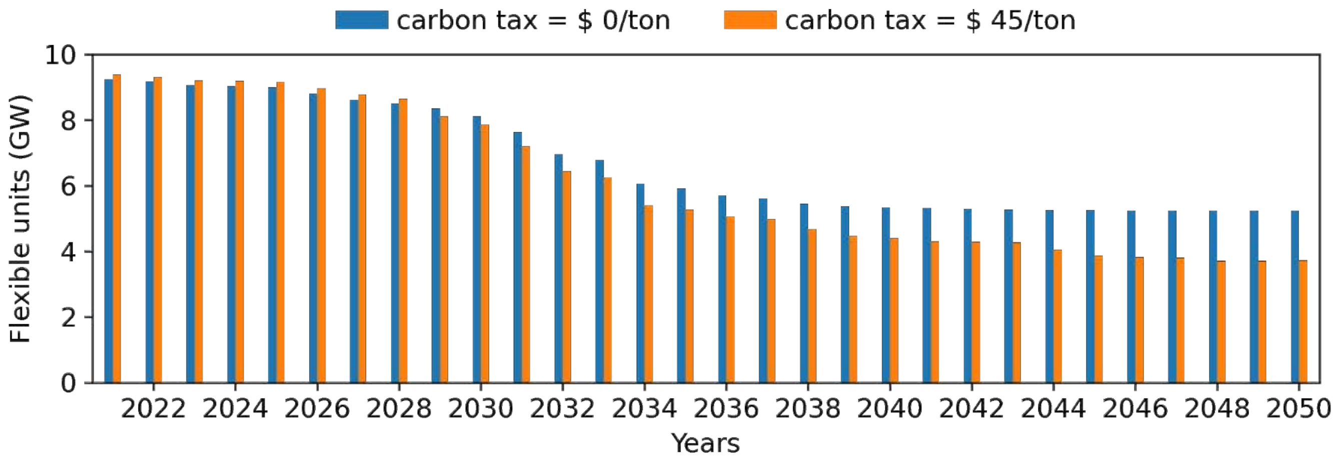
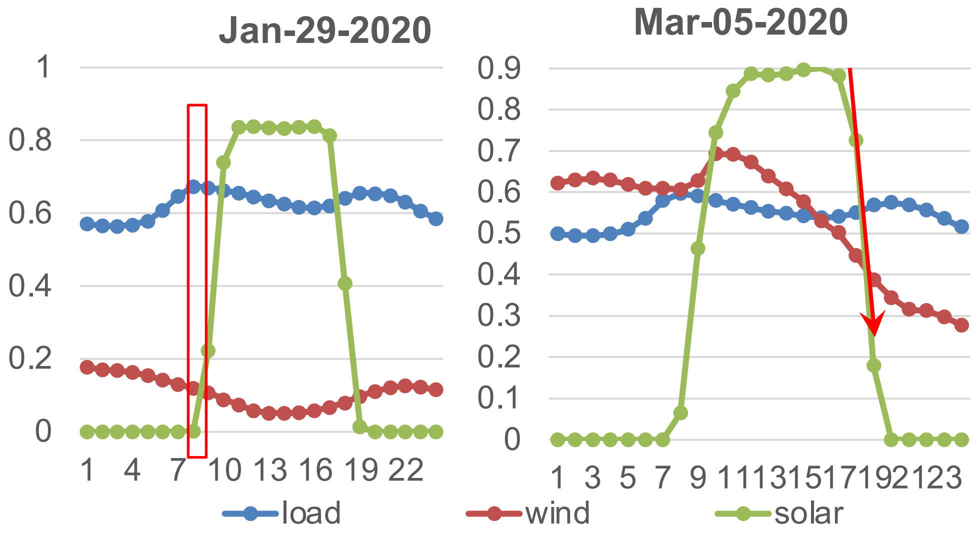
Challenge to Adequately Represent Variability with Clustering



- Expansion planning with SPP case study
  - Results indicated significant reduction of installed flexible generation
    - Gas turbine, internal combustion turbine units
    - Lower efficiency, higher relative emissions
  - *Counter-intuitive result*

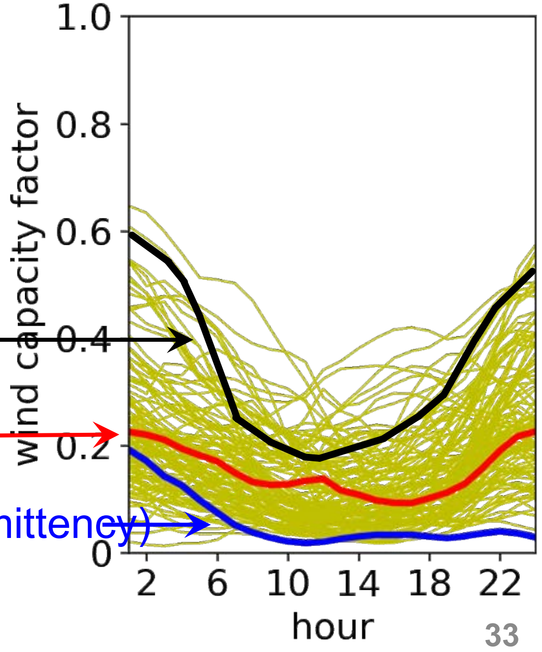
- Root cause: "representative" days did not capture
  - High ramp rates (volatility)
  - Low non-dispatchable generation (intermittency)



Scenario with high ramp rates (volatility)

Representative day

Scenario with low generation levels (intermittency)



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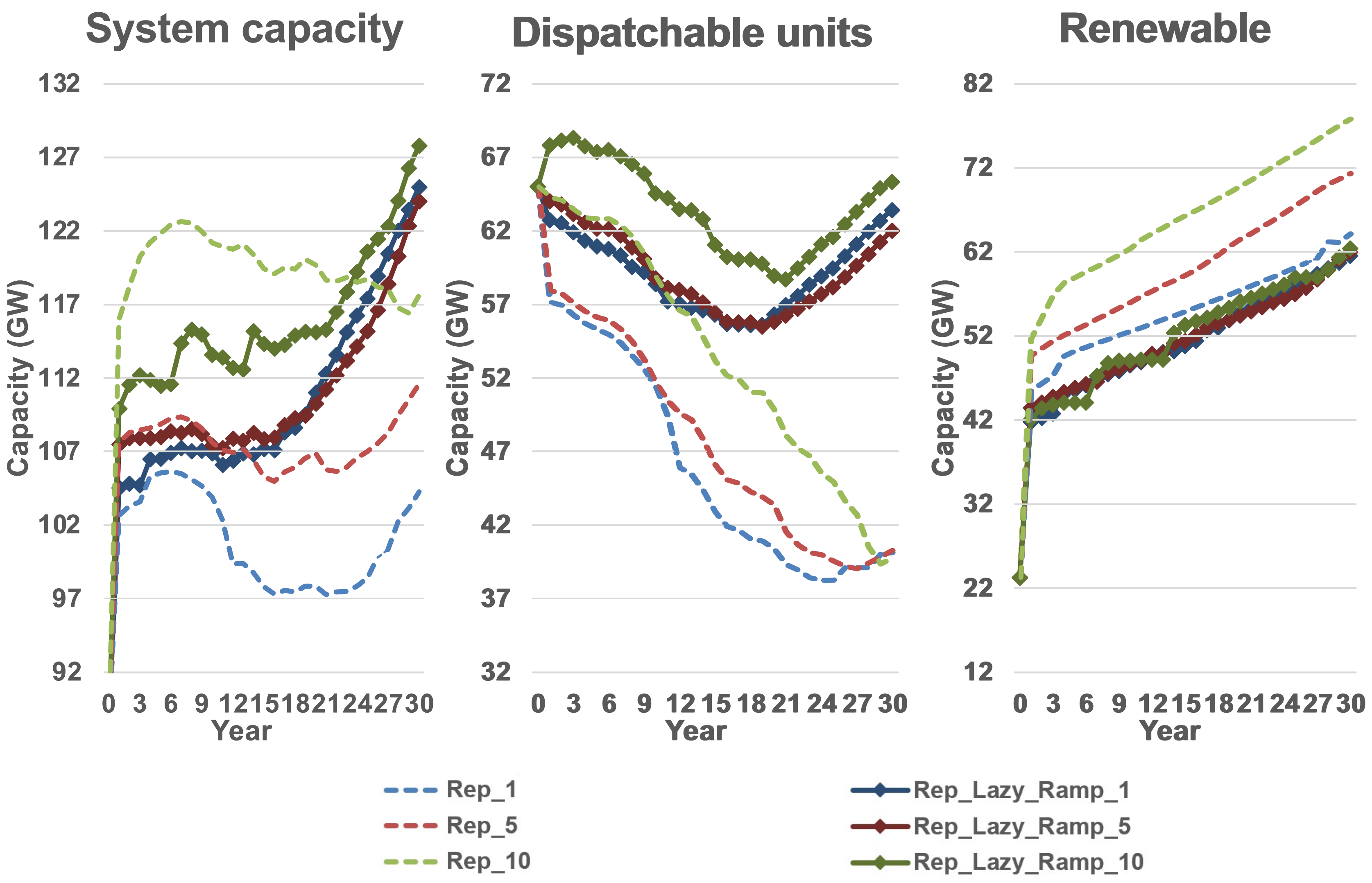
Dispatchable Plants Critical with Increased Renewables



- "Representative Days Only" underestimates total required capacity
- More dispatchable capacity required with lazy capacity constraints and ramp events
- Extreme ramp integration limits expansion of renewable capacity

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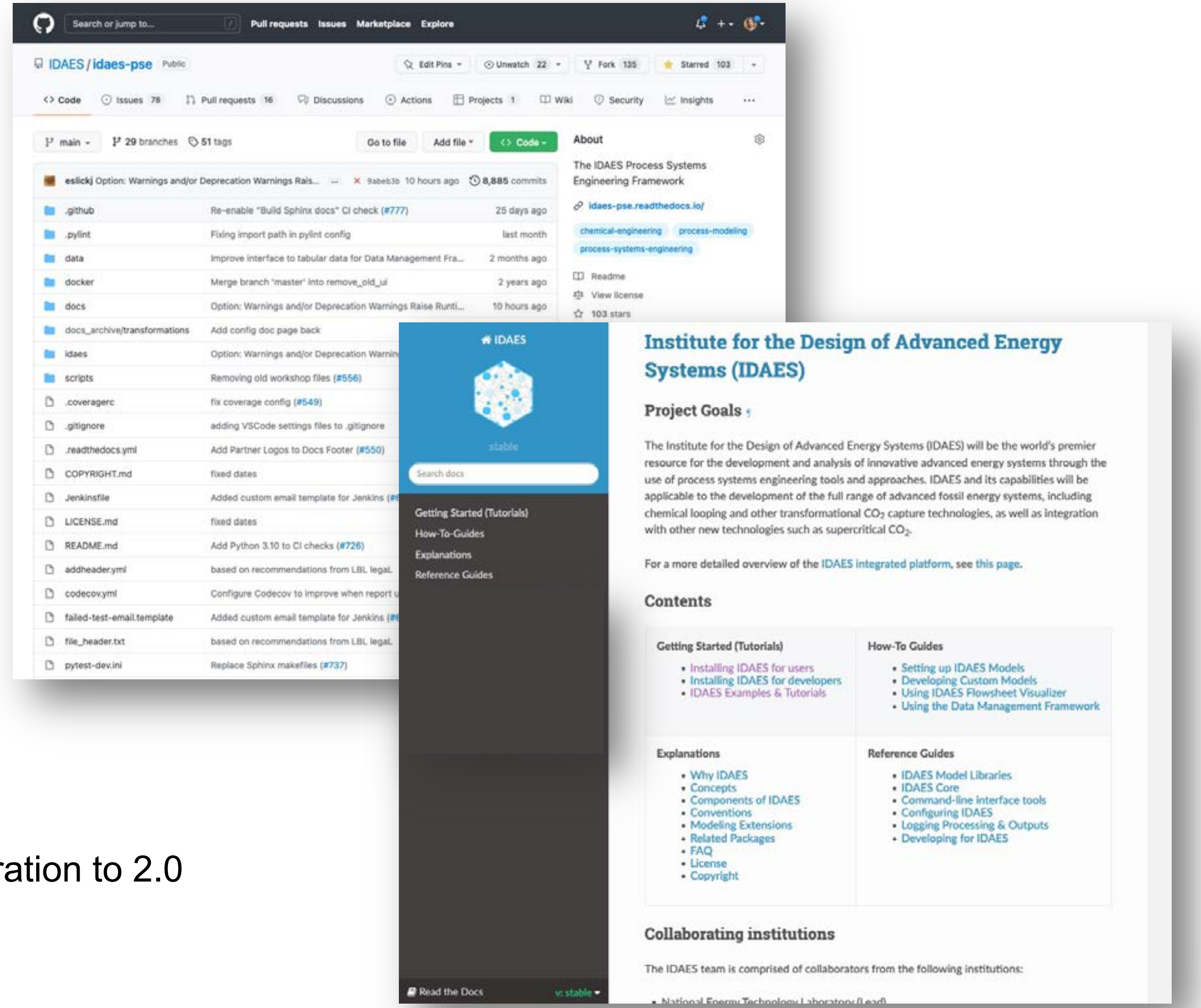
Software Development & Release Management

Mature Software Development, Test & Release Processes

- **Open-Source Software repository at GitHub**
  https://github.com/IDAES/idaes-pse
- **Continuous development, testing & documentation updates**
- **Quarterly release schedule**
  - 22 Releases in past 4 years on the 1.X line
- **2.0 Release schedule for November 2022**
  - Major organizational and API improvements
  - As learned over the past years of development
- **February's 1.13 release last of the 1.X line**
  - May & August will each have 2.0.0 alpha releases to ease migration to 2.0



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Open Source Platform

Website: https://idaes.org/

GitHub repo: https://github.com/IDAES/idaes-pse

Support: idaes-support@idaes.org

Ask questions, subscribe to our user and/or stakeholder email lists

Documentation: https://idaes-pse.readthedocs.io

Getting started, install, tutorials & examples

Overview Video

https://youtu.be/28qjcHb4JfQ

Tutorial 1: IDAES 101: Python and Pyomo Basics

https://youtu.be/_E1H4C-hy14

Tutorial 2: IDAES Flash Unit Model and Parameter Estimation (NRTL)

https://youtu.be/H698yy3yu6E

Tutorial 3: IDAES Flowsheet Simulation and Optimization; Visualization Demo

https://youtu.be/v9HyCiP0LHg

Summary

- **Trends Requiring Innovation in Decision Support Tools Multi-scale optimization**
  - Evolving energy ecosystem requires greater flexibility
  - Expanding and decarbonizing U.S. industry
  - Process intensification & modularization
  - Integrated energy systems (Hybrid approaches)
  - Tighter coupling across temporal and spatial scales/domains
- **Need for Advanced, Optimization-Based Modeling Platform**
  - Decision support for nonlinear, interacting dynamic systems
  - Multi-Scale from molecular to process/plant to enterprise
  - Leverage 30 years of progress in algorithms, hardware, modeling
- **Examples of IDAES Optimization Approach**
  - Process/Grid Coupling
  - Technical risk reduction for scaling up and deploying new technologies
  - Flexible Carbon Capture System Design
  - Integrated Energy System Design
  - Expansion Planning

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

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GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

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NAWI National Alliance for Water Innovation
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