Optimizing Innovative Energy Systems of the Future

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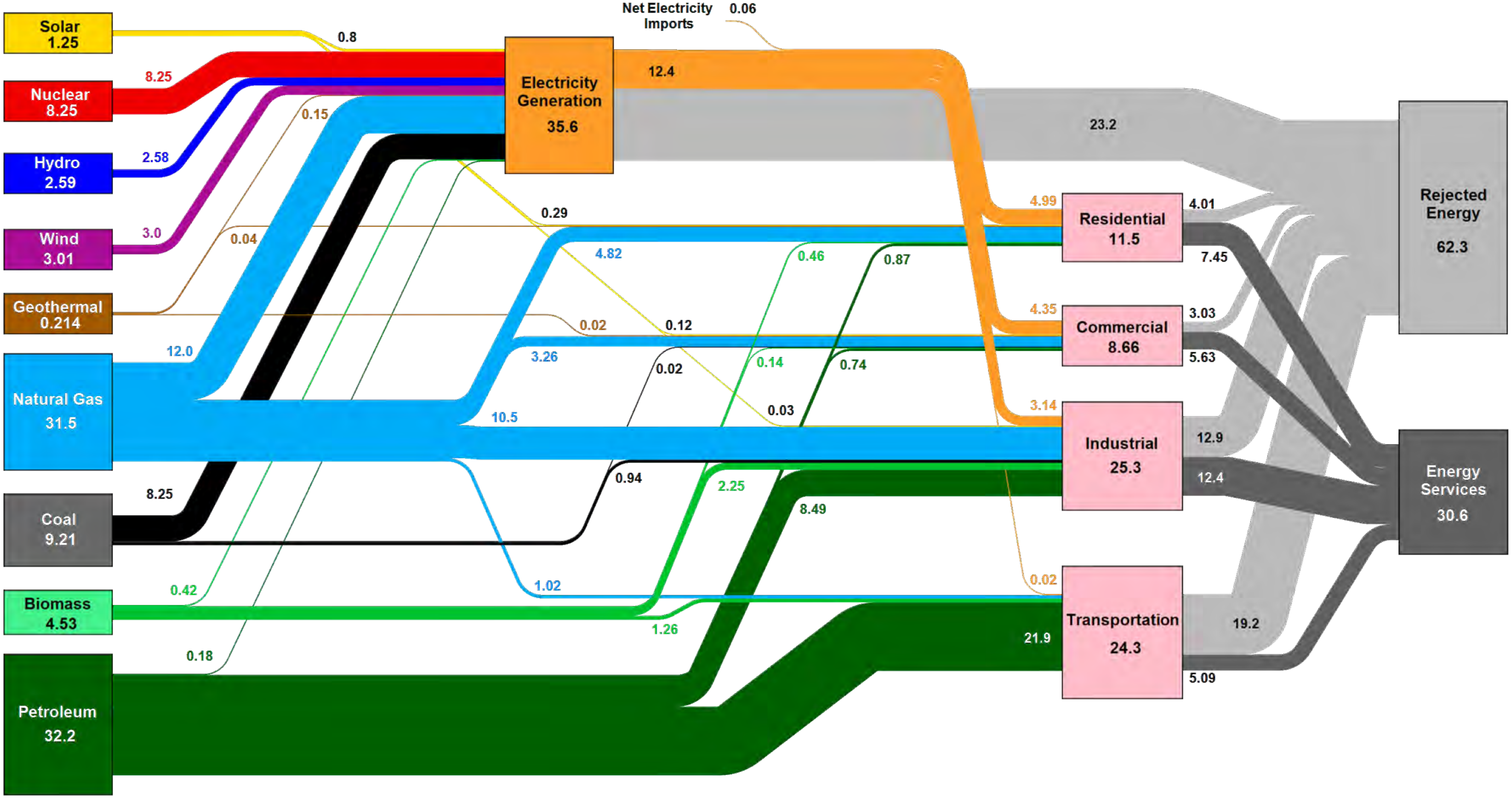
Estimated U.S. Energy Consumption in 2020: 92.9 Quads

Lawrence Livermore National Laboratory



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

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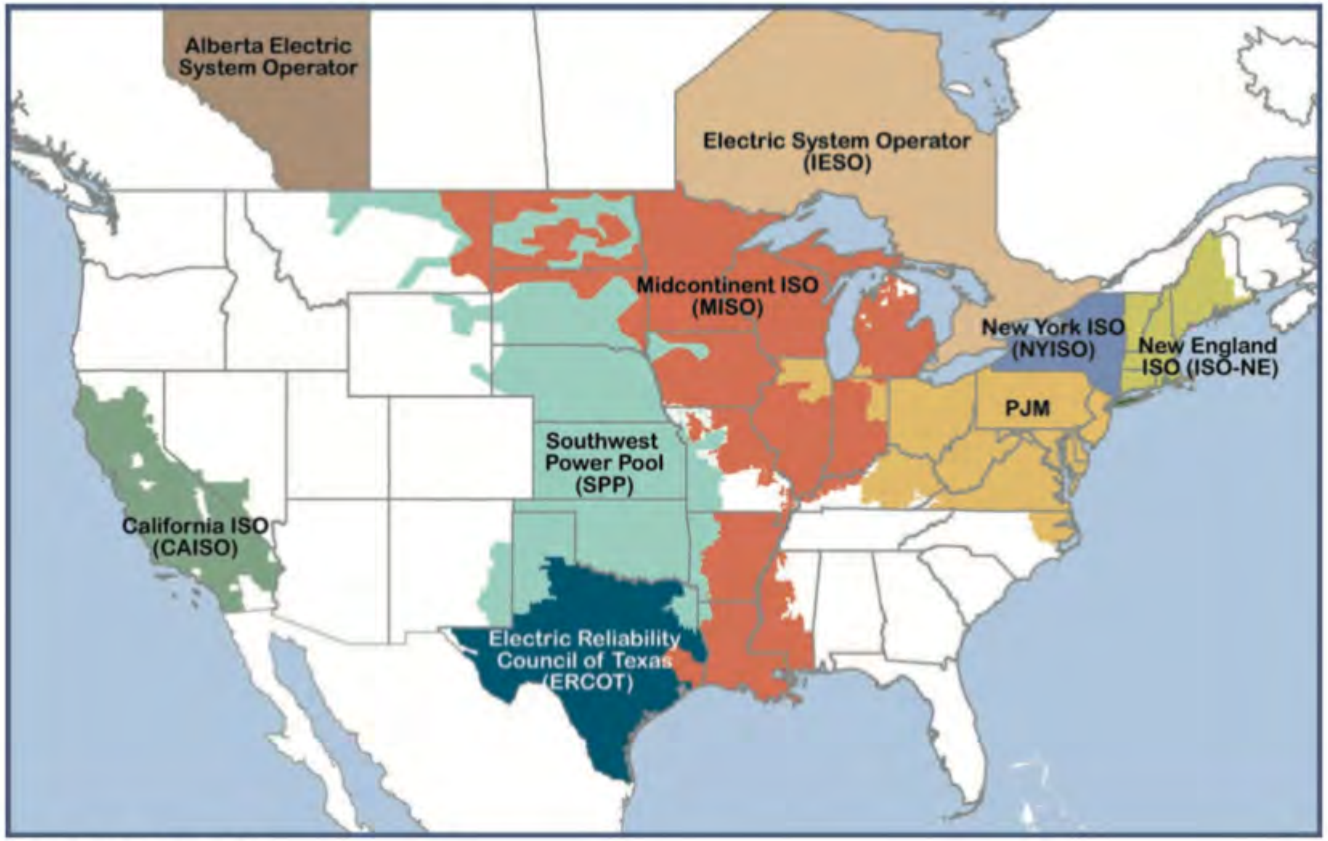
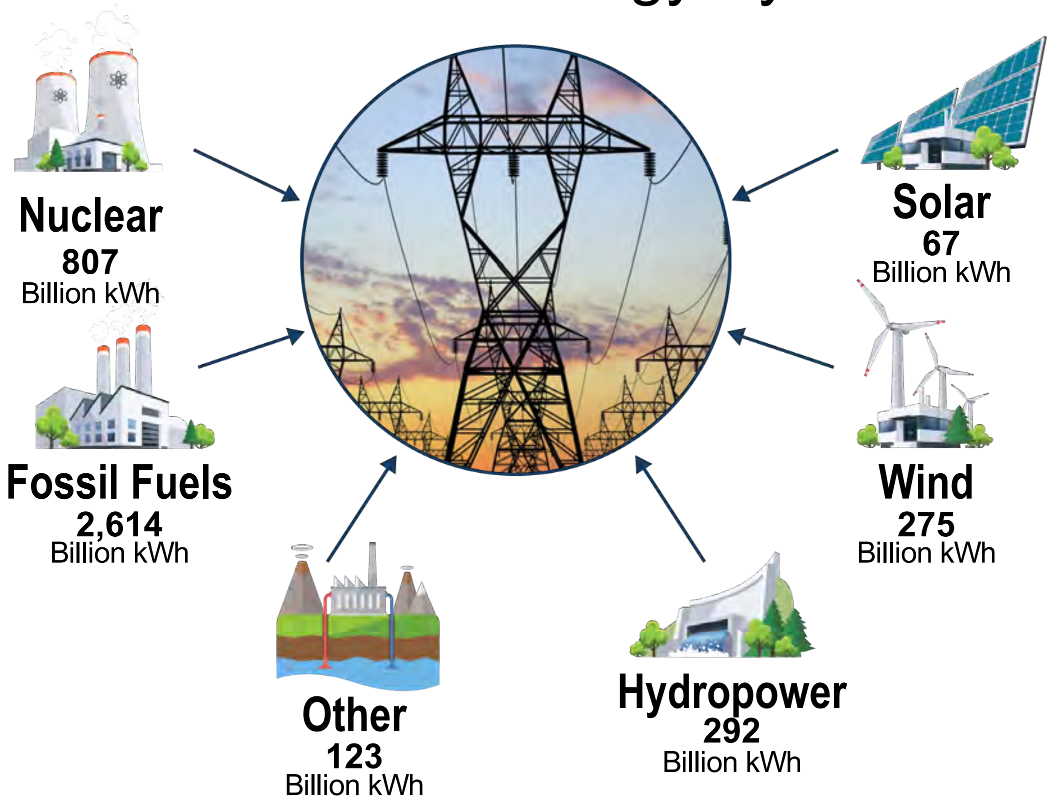
An Evolving Energy Ecosystem

North American Independent System Operators and Regional Transmission Organizations



Source: Velocity Suite, ABB

Coordinated Energy System



Total: 4,178 Billion kilowatt-hours (kWh)

Data source: EIA, 2018

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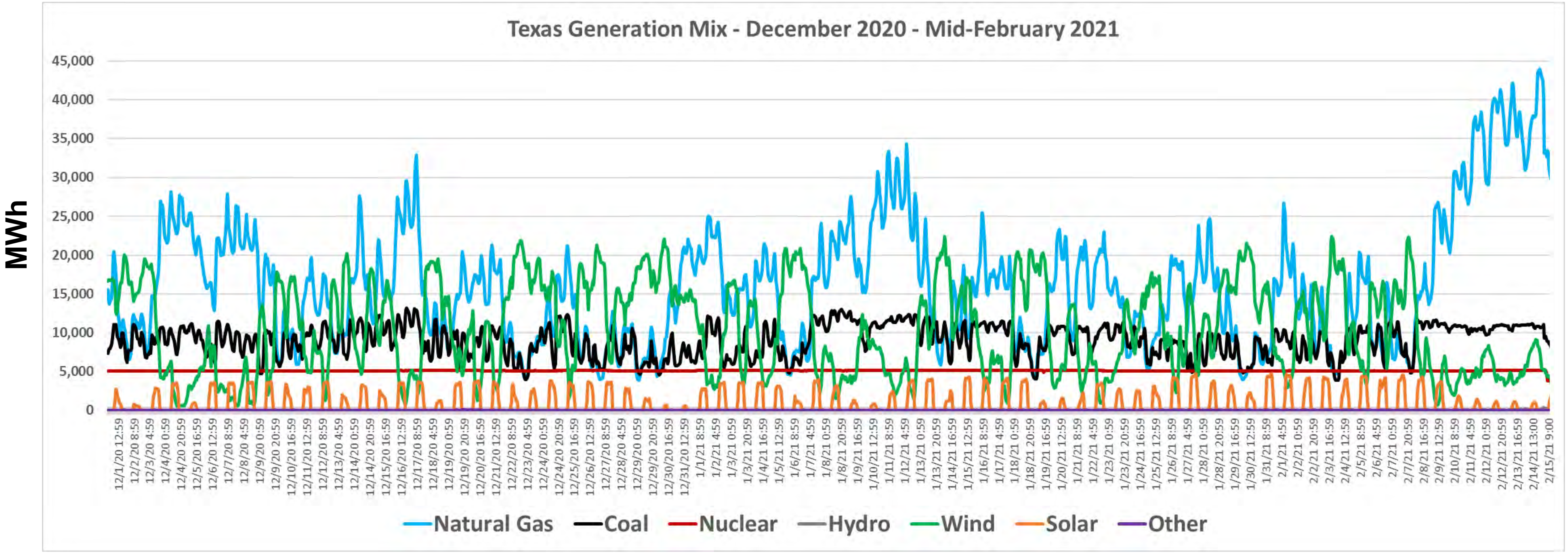
Variability in Electricity Production Requires Flexibility



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Expanding U.S. Industry & Chemicals Production

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

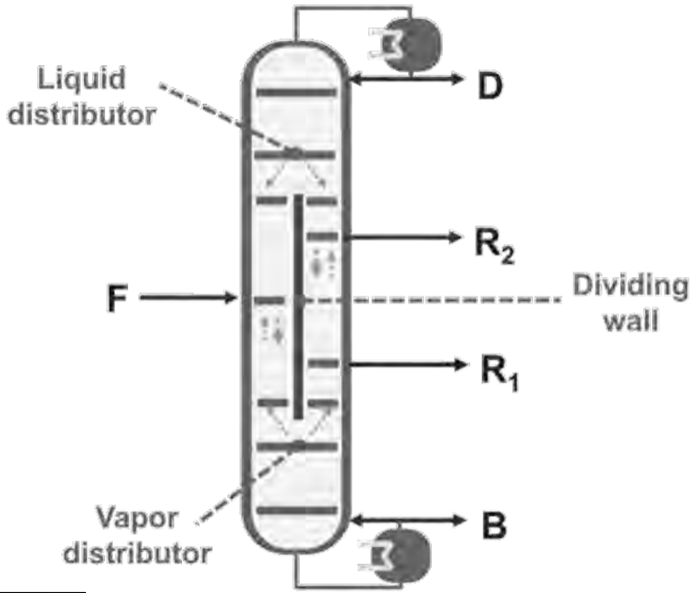
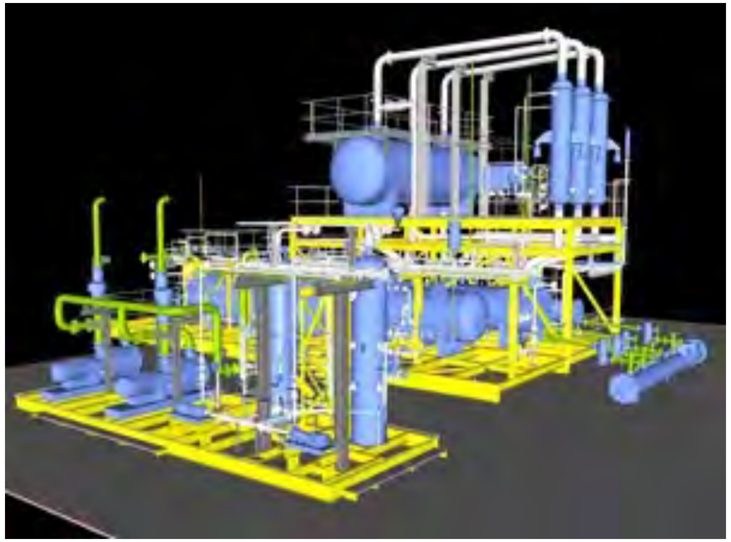
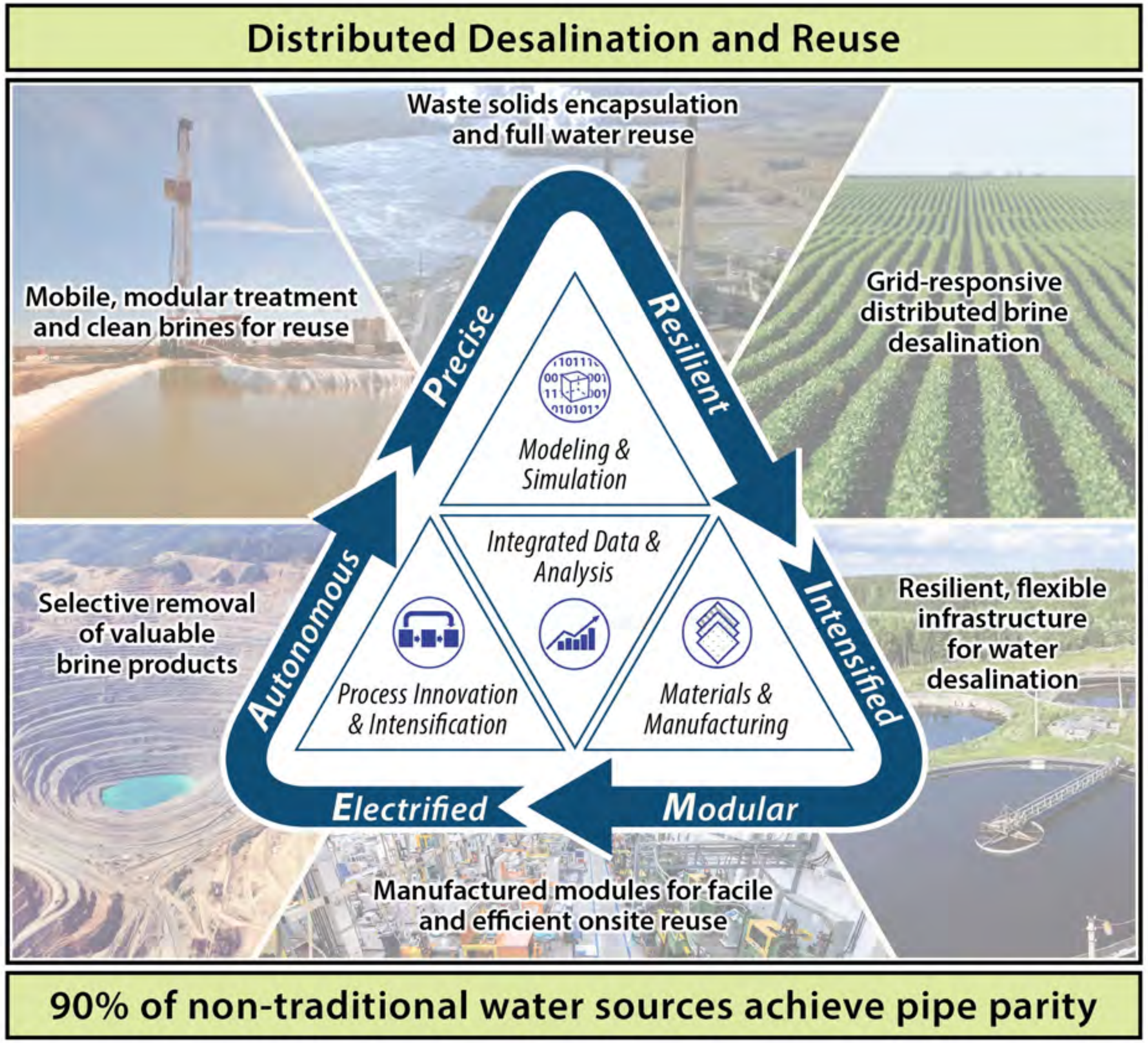


Figure from Rawlings et al., 2019



Non-traditional Water Sources Require Innovation



- New operating paradigms
  - Distributed
  - Grid responsive
  - Dynamic
- New treatment technology
  - Innovation, intensification
  - New materials
- Multiple source waters
  - Robust designs
  - Rapid reconfiguration

National Alliance for Water Innovation

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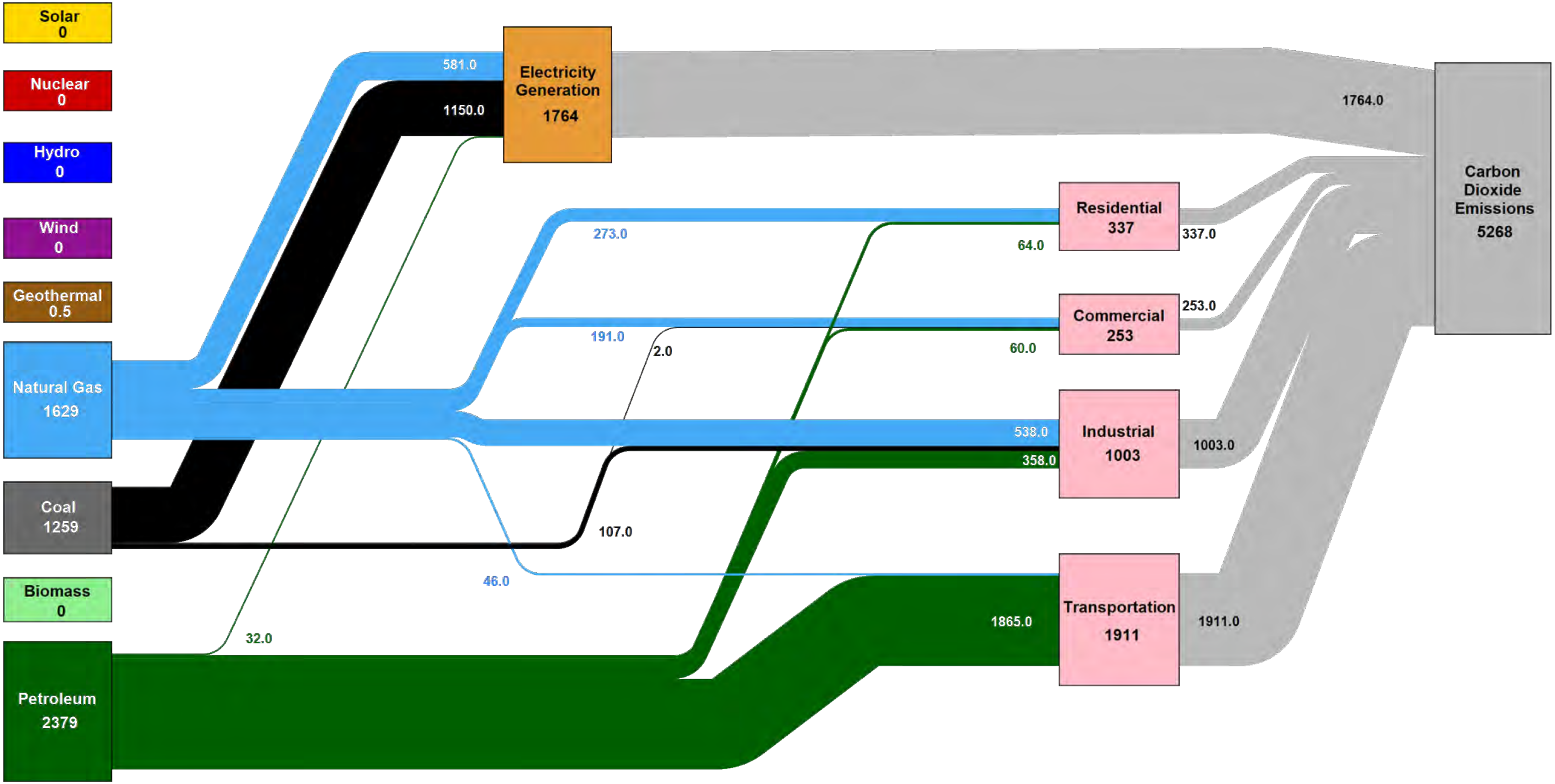
Estimated U.S. Carbon Dioxide Emissions in 2018: ~5,268 Million Metric Tons

Lawrence Livermore National Laboratory



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 residential, 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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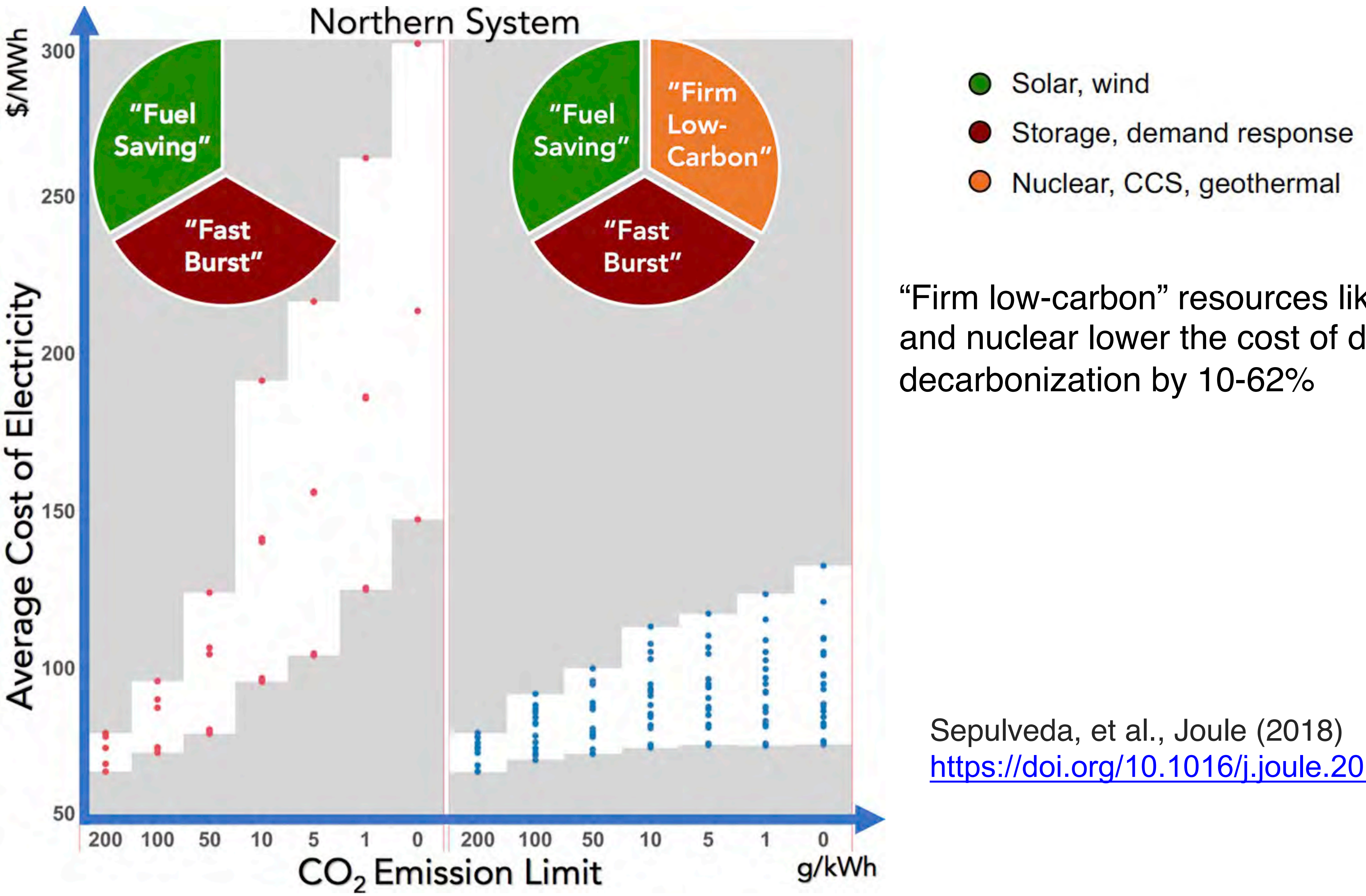
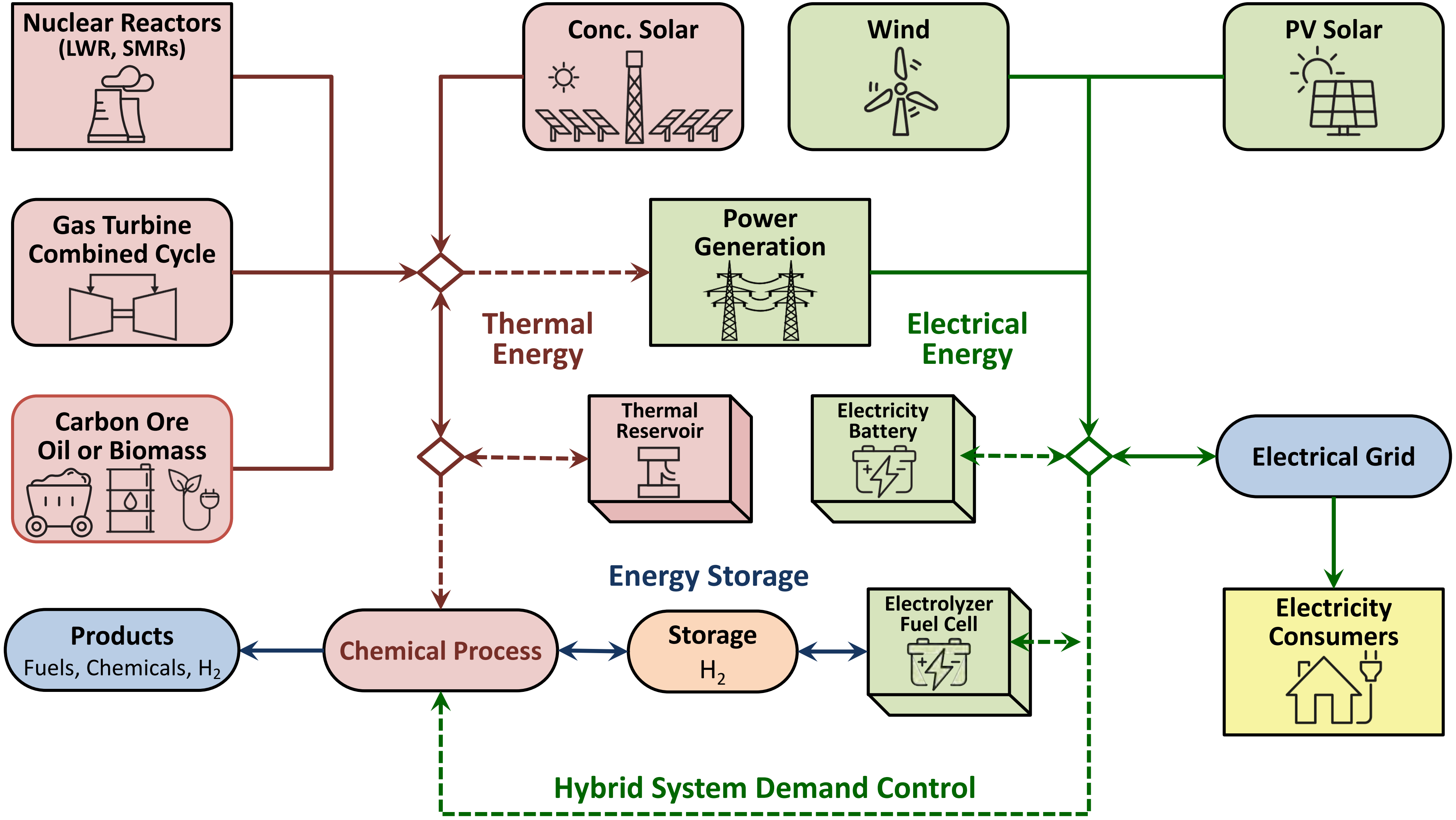
Need for Dispatchable Power for Economic Deep Decarbonization



"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

Integrated Energy Systems Expand Design & Operations Space



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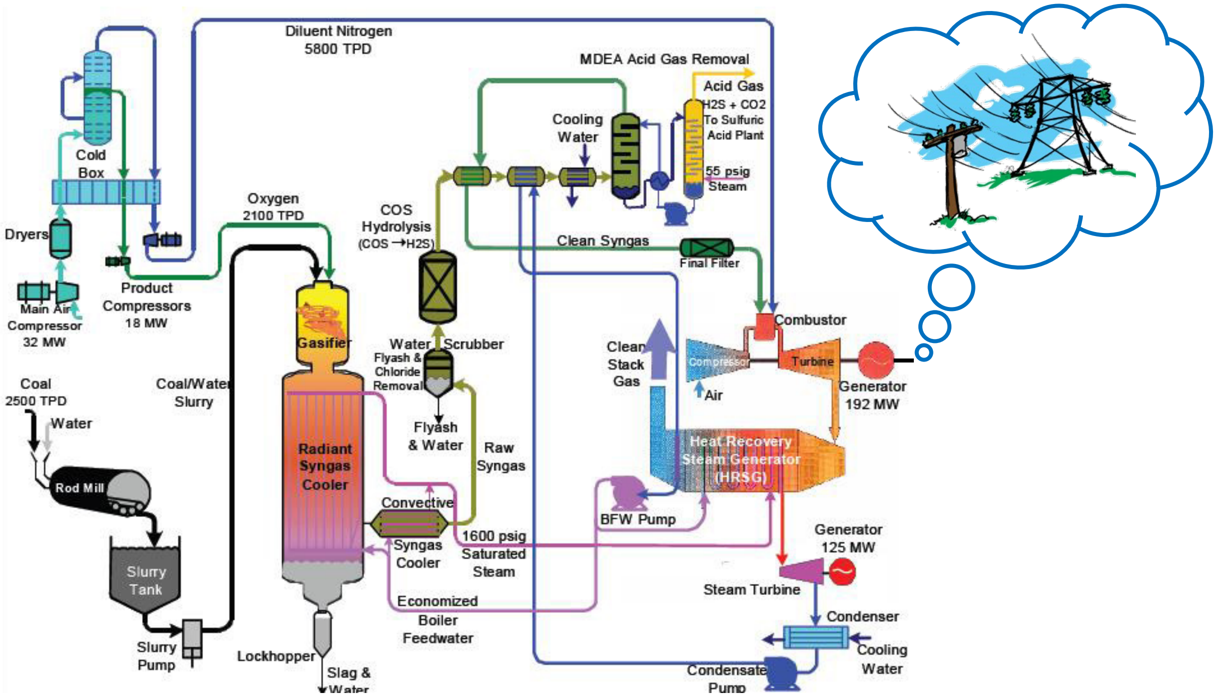
Energy System Analysis is Often Applied in Isolation

Process-centric Modeling

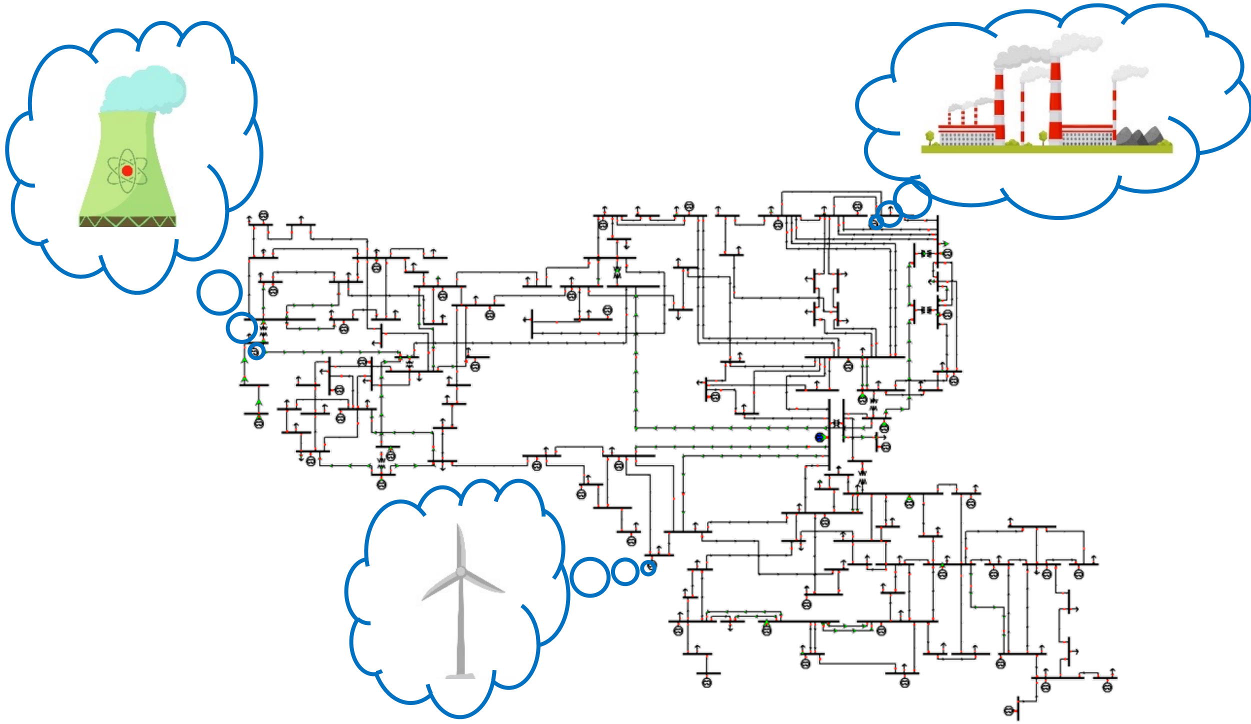
Detailed steady state or dynamic process models, with the grid modeled as an infinite capacity bus



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"



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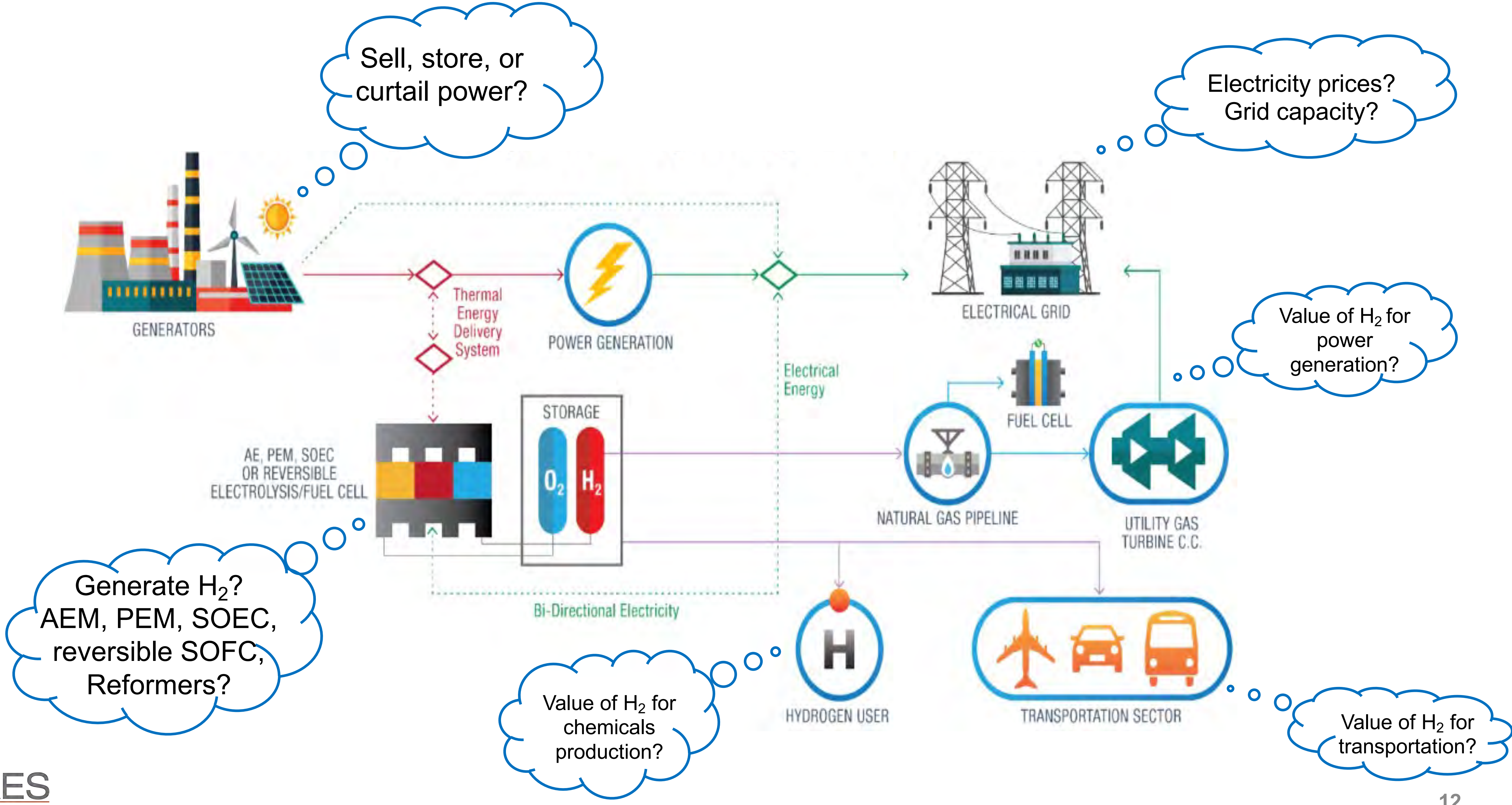
From Dowling et al. (2020)

Integrated Energy System For Power and H_2 Production



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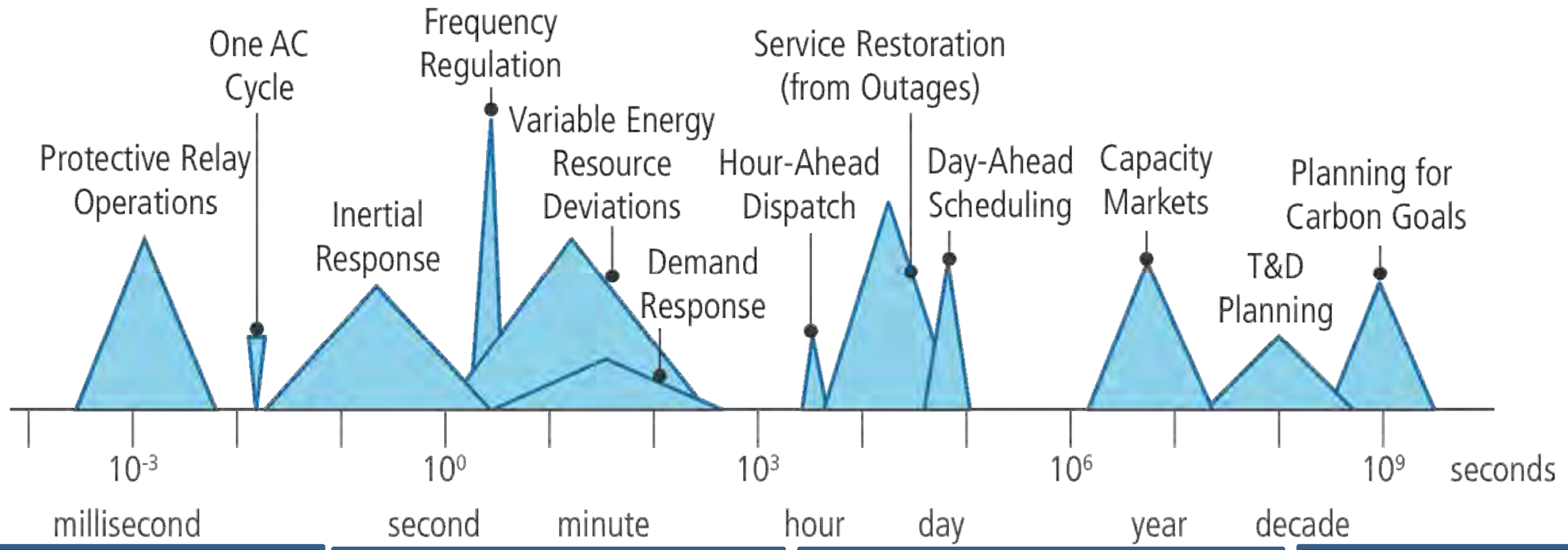
Multiple Time Scales & Perspectives Across Tools



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

Trends Requiring Innovation in Decision Support Tools

- Evolving energy ecosystem requires greater flexibility
- Expanding U.S. industry
- Process intensification & modularization
- Treatment & desalination of non-traditional water sources
- Integrated energy systems (Hybrid approaches)
- Tighter coupling across temporal and spatial scales/domains

Requirements for Advanced Modeling Platform

- Decision support for nonlinear, interacting systems: **Optimization Focus**
- Multi-Scale from molecular to process/plant to enterprise
- Dynamic optimization
- Enable Innovation
- Reusable Building Blocks
- Flexible & Customizable
- Leverage 30 years of progress in algorithms, hardware, modeling

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

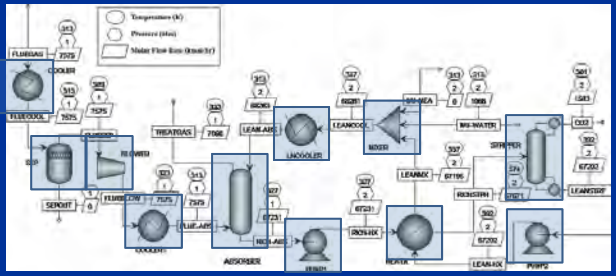
Optimization over degrees of freedom only

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

u

f

Simulator



Black-box optimization (DFO)
~ 100-1000 simulations

Glass-box optimization
~ 1-5 STE

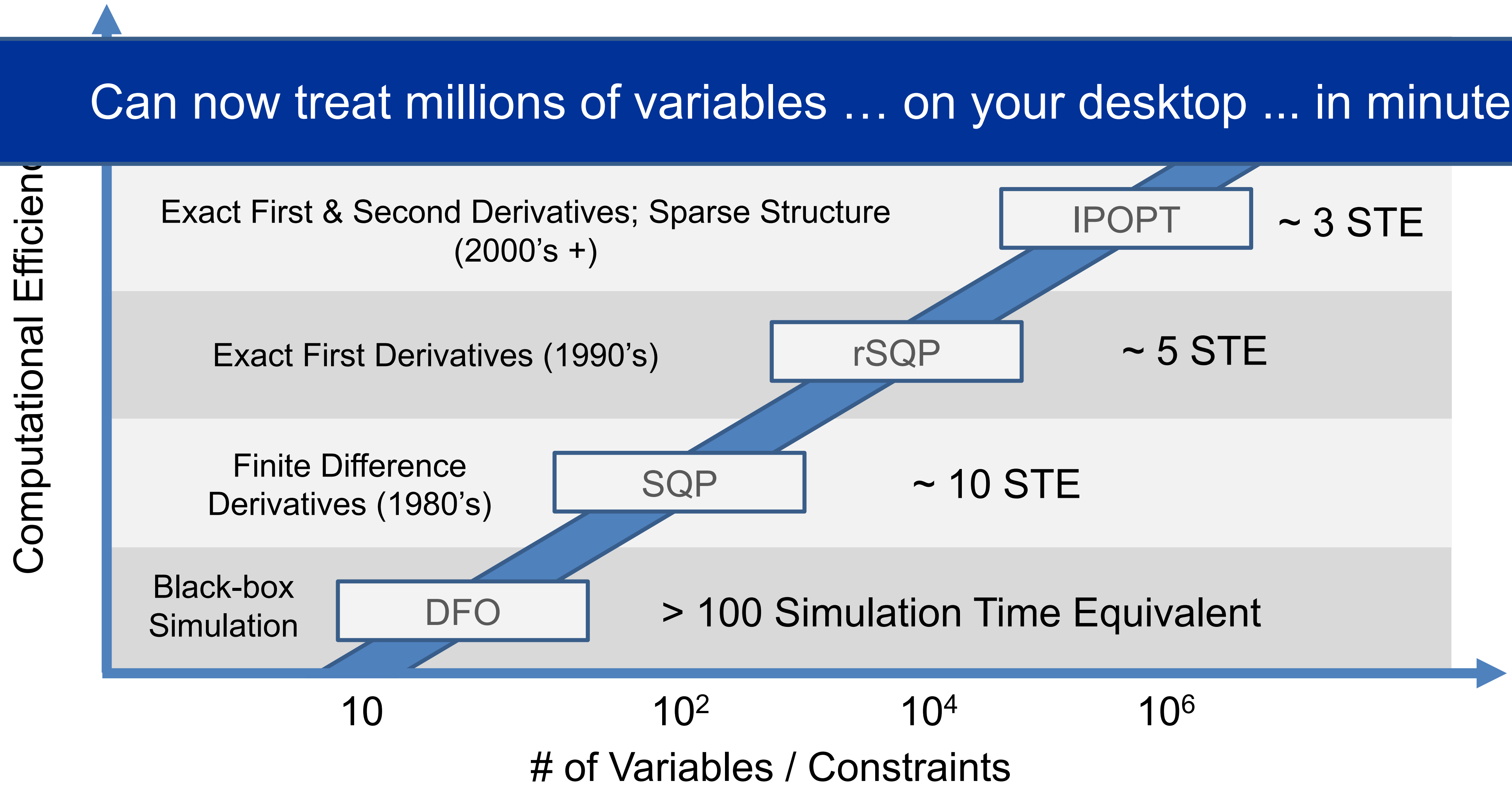
Optimization with embedded algebraic model as constraints

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

[Adapted from Biegler, 2017]

Process Optimization Environments and Nonlinear Solvers

Can now treat millions of variables … on your desktop ... in minutes



[Adapted from Biegler, 2017]

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IDAES Integrated Platform

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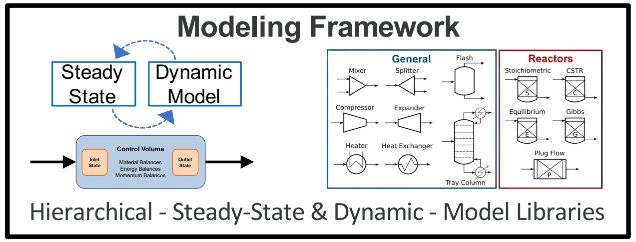
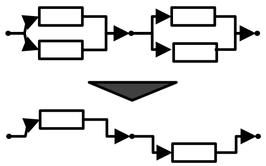
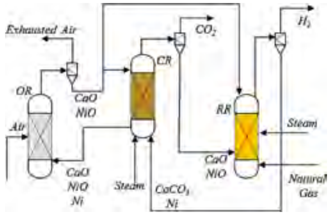


Conceptual Design



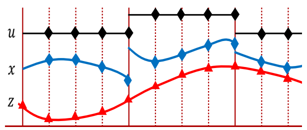
PYOMO GDP

Plant Design
Process Optimization



Process Operations
Dynamics & Control

caprese



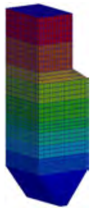
Uncertainty Quantification
Robust Optimization

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

2020 R&D 100 WINNER

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Carnegie Mellon

West Virginia University

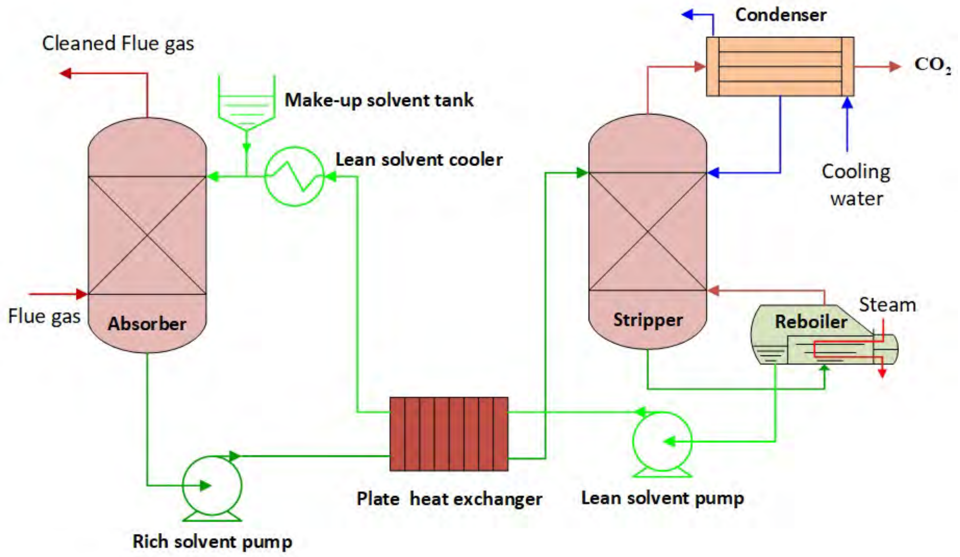
UNIVERSITY OF NOTRE DAME

PYOMO

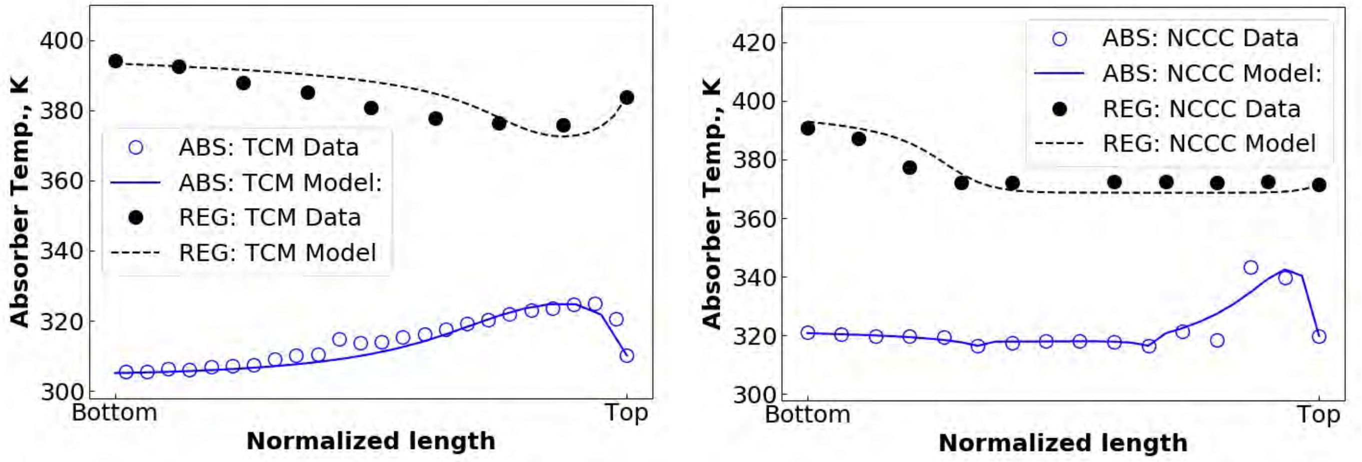
python™

Gurobi	CPLEX	Xpress	CBC	Ipopt
GAMS	NEOS	Mosek	BARON	GLPK

Advanced Models for Solvent-Based CO_2 Capture

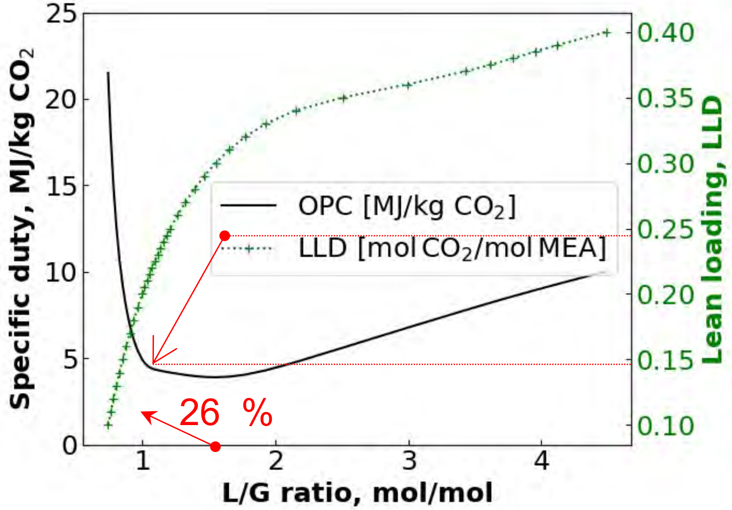


Model Validation



- Modular, multi-scale, dynamic rate-based
- Film model: multi-component mass and heat transport
  - Simultaneous reaction & transport of molecular & ionic species
- Rigorous properties
  - Modified eNRTL model for mixed solvent systems
- Plant-wide model enables complex optimization

Process Optimization



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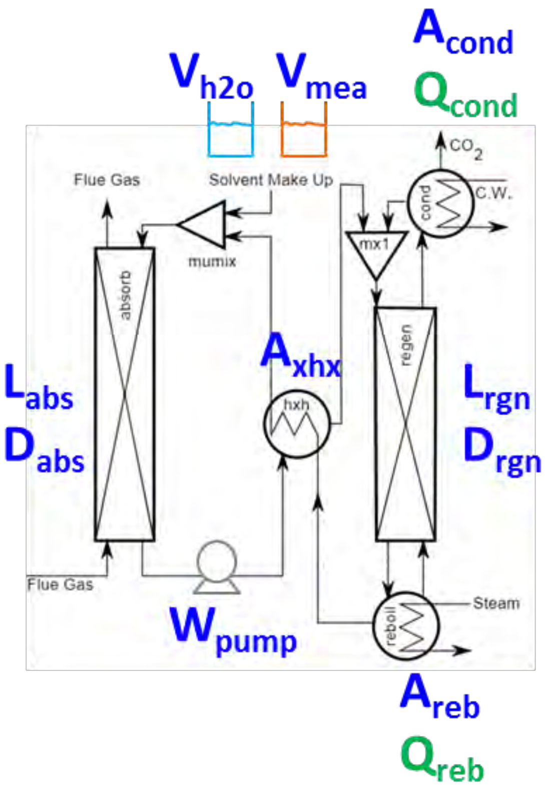
Robust Design to Reduce Technical Risk

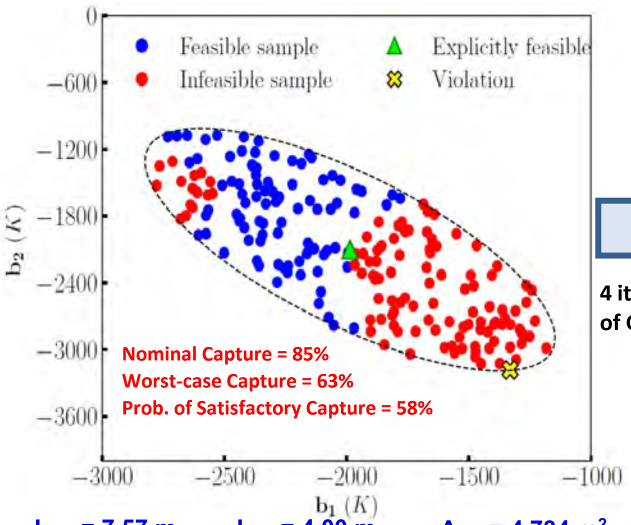
Inherent uncertainty in process design models

- 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

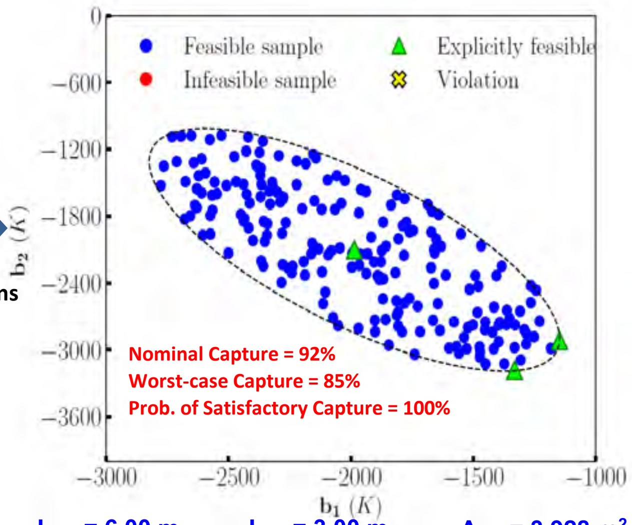


L_{abs} = 7.57 m
D_{abs} = 4.95 m
L_{reg} = 4.00 m
D_{reg} = 3.44 m
A_{xhx} = 4,734 m^2
Q_{reb} = 18 MW
Q_{con} = -4.5 MW

4 iterations of GRCS

Robust Solution

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



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*

Optimizing Flexible System Design to Respond to LMP Signals

- Design a flexible carbon capture system for power plants to operate in a high VRE grid
- Different scenarios based on carbon prices, regions
- Resulting problem is a multi-period stochastic optimization problem

$$\max_{d,u} NPV = \sum_{s \in S} w_s f(Revenue - Capital\ Cost - Operating\ Cost)$$

$$\sum LMP_t * Power_t$$

- LMP signal from ARPA-E
- Scenarios will be considered independently

$$\sum \begin{matrix} TSA(design\ variables) + \\ CO_2\ compression\ (design\ variables) \end{matrix}$$

- Capital costs only for capture system

$$\sum \begin{matrix} NGCC(operating\ variables) + \\ TSA\ (operating\ variables) \\ + CO_2\ compression(operating\ variables) \end{matrix}$$

- Operating cost for NGCC and capture system

$+$

Model Equations $g(d, u_s, x_s) = 0, s \in S$

$+$

Design/Operating Constraints $h(d, u_s, x_s) \leq 0, s \in S$

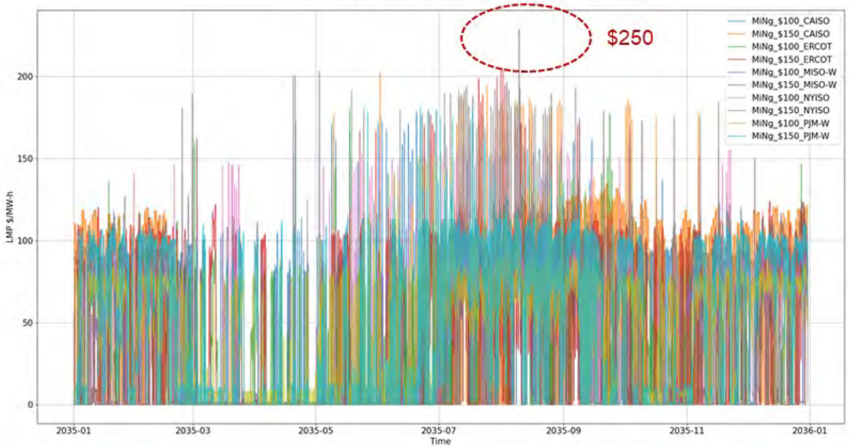
d – design (stage 1) variable

u – operating (stage 2) variable

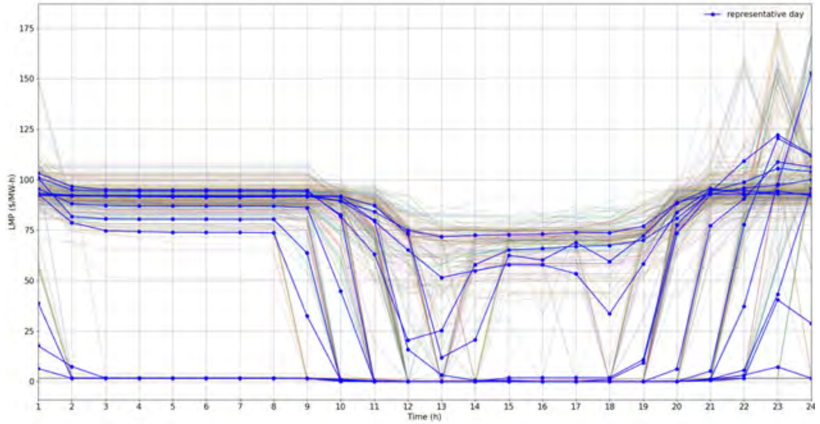
S – Finite set of scenarios (representative days)

w_s – weight for scenario s

NREL Data Set (10 scenarios)



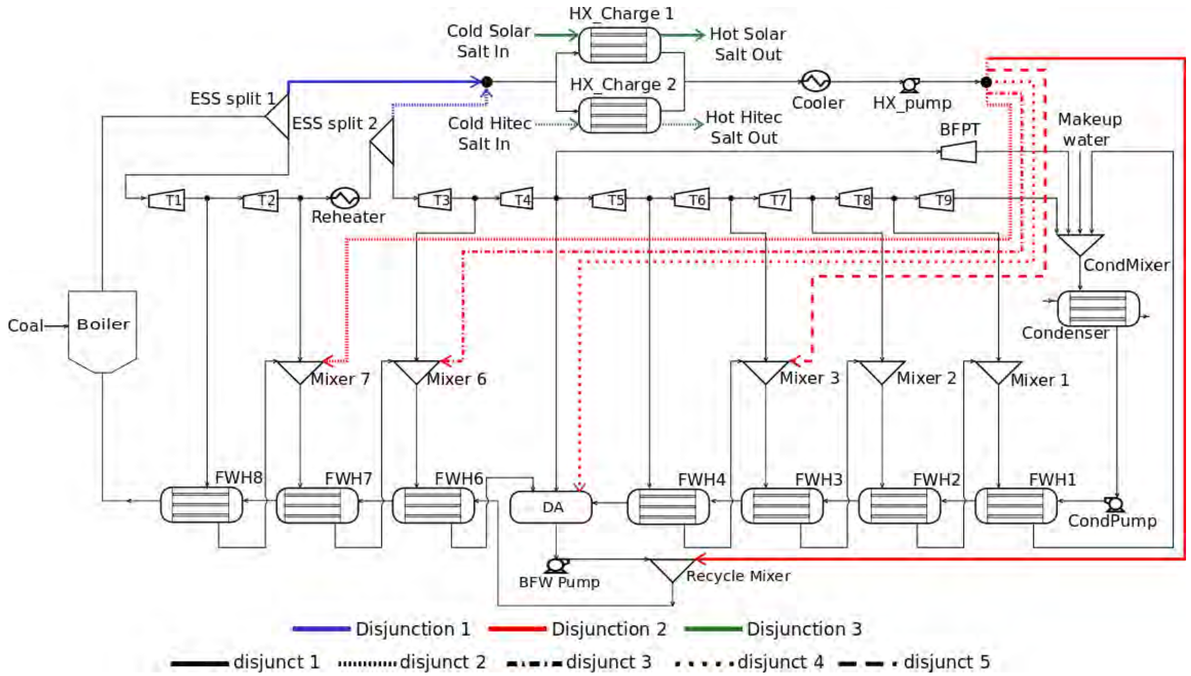
12 Representative Days



Conceptual Design of Thermal Energy Storage with GDP

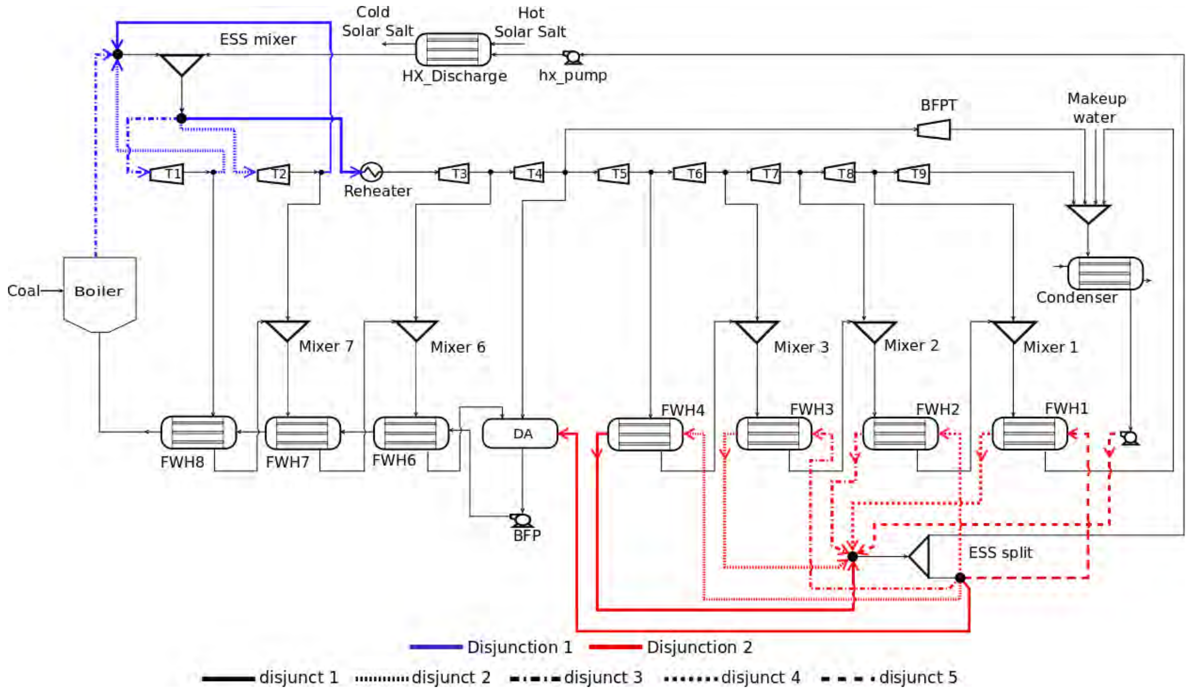
Charging Case (20 possibilities)

MIP: Gurobi, NLP: IPOPT. 572 constraints, 512 variables, 9 integer vars



Discharging Case (15 possibilities)

MIP: Gurobi, NLP: IPOPT. 532 constraints, 442 variables, 8 integer vars



Problem Specification

- Power reduced to 521 MW (baseload is 693 MW)
- 150 MW_{th} diverted to charge; 148.5 MW_{th} extracted during discharge
- System designed for 6h of charging/discharging at rated storage capacity
- Minimize total annualized cost

Implementation

- Uses IDAES unit models, IDAES costing library, and IDAES conceptual design tools
- Problem formulated as Generalized Disjunctive Programming (GDP) problem
- Able to explore several combinations with a single model
- Avoid exhaustive enumeration
- Solution time:
  - Charge - 7 mins wall time
  - Discharge – 3 mins wall time

Optimal Design

- Salt selected: Solar salt
- Charge:
  - Steam source – T3 (IP inlet)
  - Steam sink – FWH7 Mixer
- Discharge:
  - BFW source – FWH4
  - Steam sink – T2 (HP stage)

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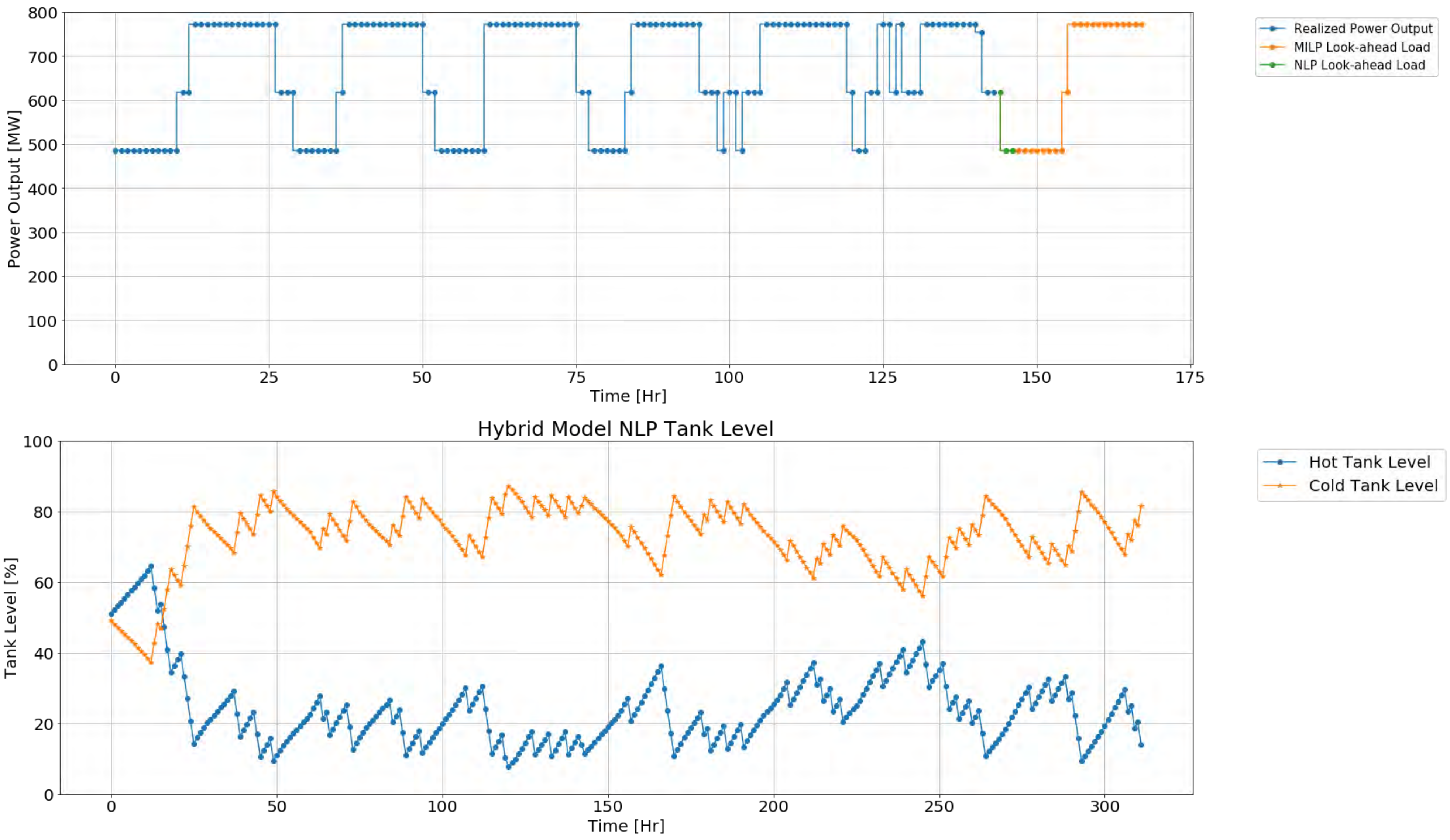
NMPC Control of Generator + Thermal Energy Storage

Tracks market dispatch signal for hypothetical thermal generator with integrated thermal energy storage



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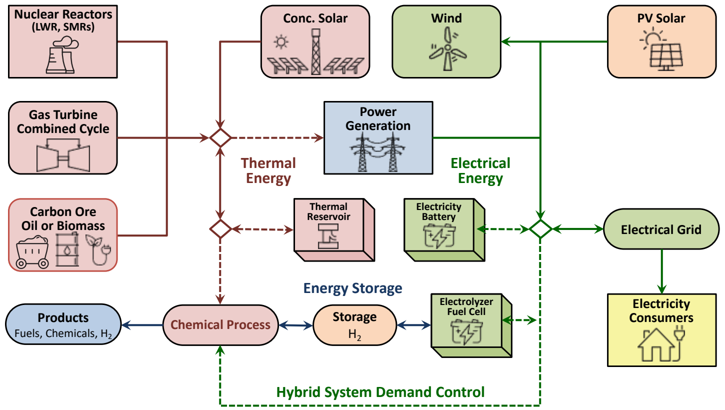
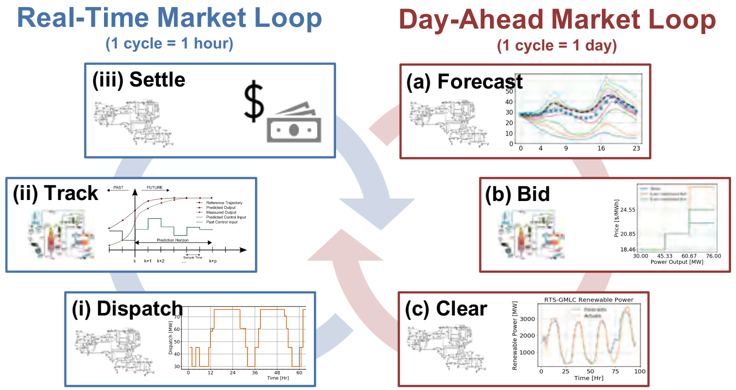
Bridging Timescales Enables Unique Analyses & Design of IES

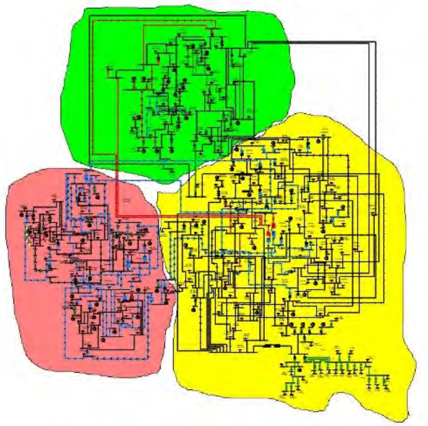
High-Fidelity Process Modeling



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

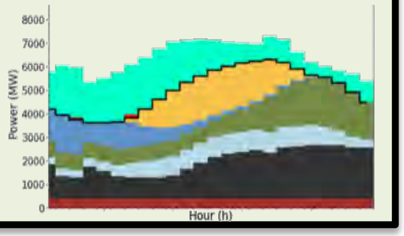
Market Surrogates Enable Conceptual Design

1.) Define system search space

Defines simulation space

2.) Perform market simulations

PRESCIENT



>68,000 simulations link generator parameters to market outcomes

3.) Train surrogate models to map generator characteristics to market outcomes

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ALAMO
a black-box modeling tool

Surrogate models predict market outcomes given generator decisions

4.) Define and solve superstructure optimization problem to determine optimal design

Best candidate designs

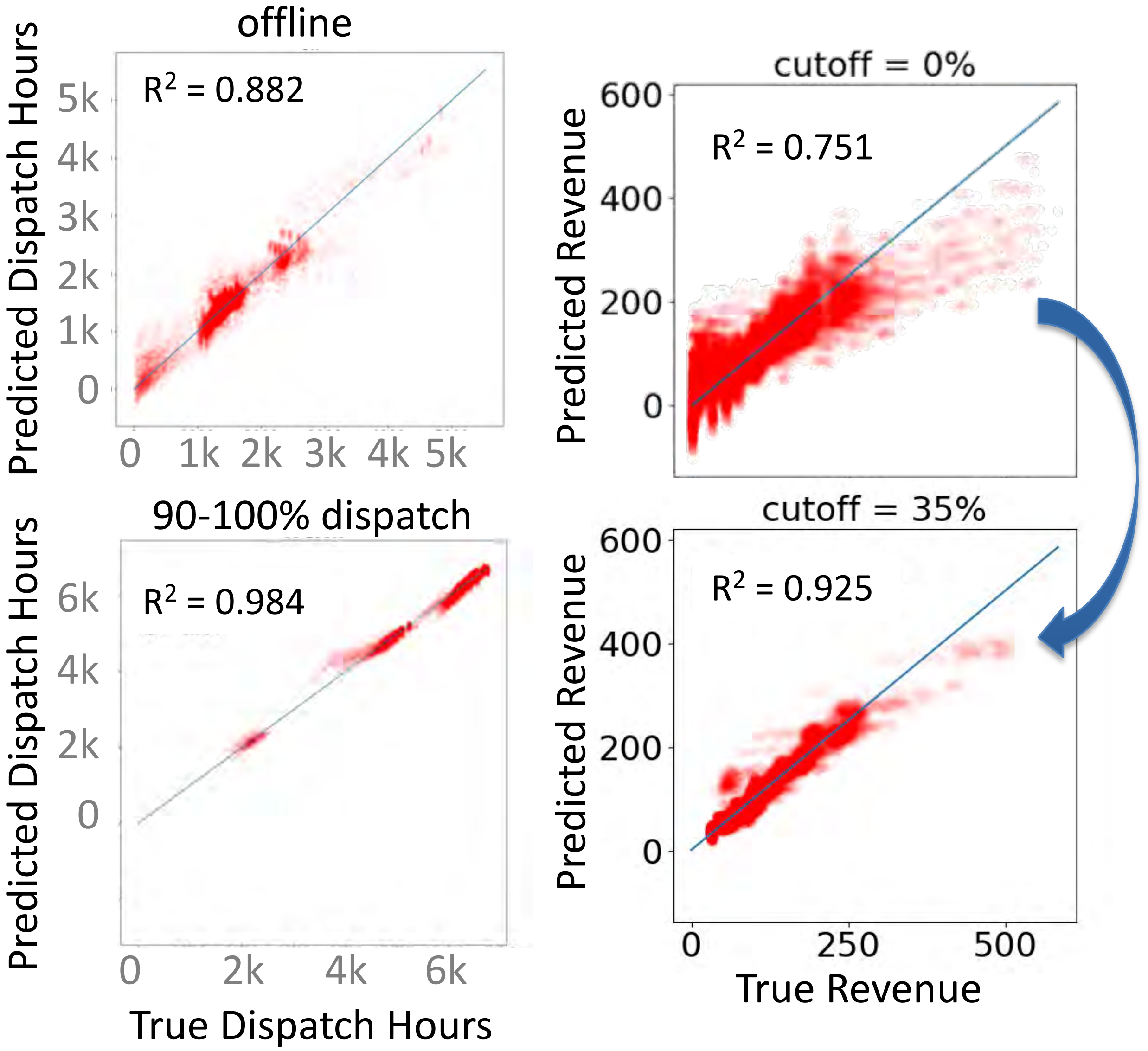
5. Simulate optimal participation of candidate designs in electricity markets

Optimal market outcomes over annual time horizon.

6. Verify results are consistent with surrogate models

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

Scalable Conceptual Design with Market Interaction Surrogates



Conceptual Design (Step 1)

Maximize Profit

$$\max_{d,u_s} \; R(x) - \sum_{s \in S} w_s(x) C(d, u_s, \delta_s)$$

Plant Constraints

$$s.t. \quad g(d, u_s, \delta_s) = 0, \quad s \in S$$

$$h(d, u_s, \delta_s) \leq 0, \quad s \in S$$

Satisfy Demand, Link Design to Market Inputs

$$\delta_s = g_1(d, u_s)$$

$$g_2(d, x) = 0$$

Surrogate models

Revenue & Fraction of Dispatch

$$R(x) = f_{\text{revenue}}(x)$$

$$w_s(x) = f_{\text{dispatch}}(x), \quad s \in S$$

Optional cutoff constraint

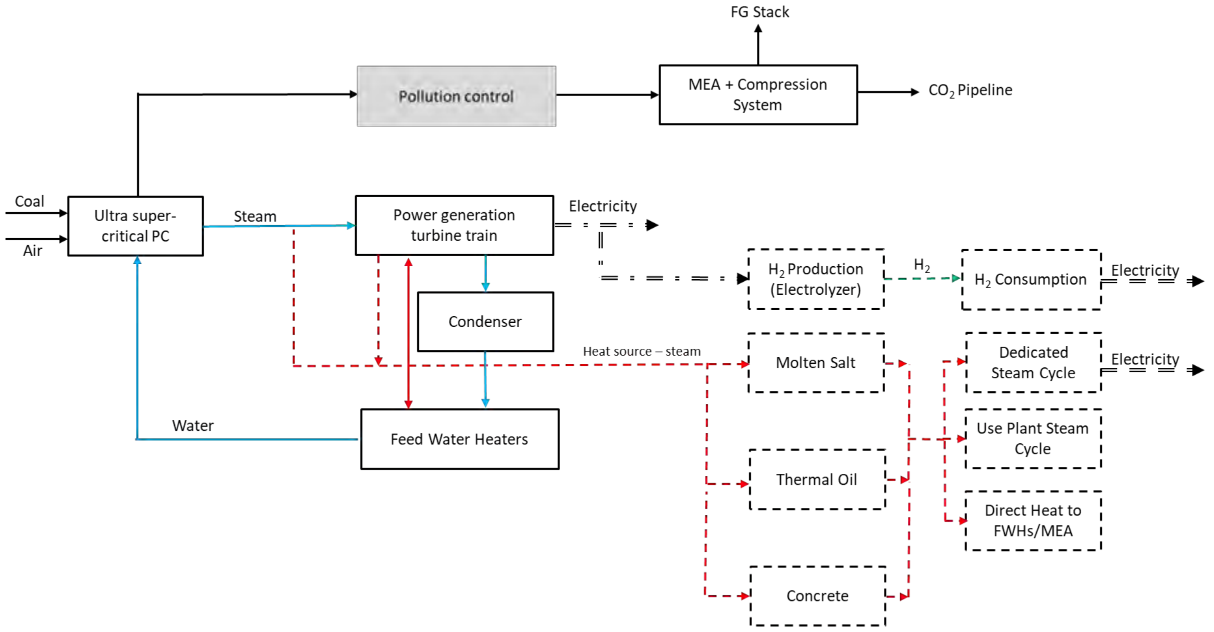
$$\text{cutoff}(x) = \sum_{i \in SV} y_i \lambda_i x_i^T x + b \geq 0$$

DISPATCHES

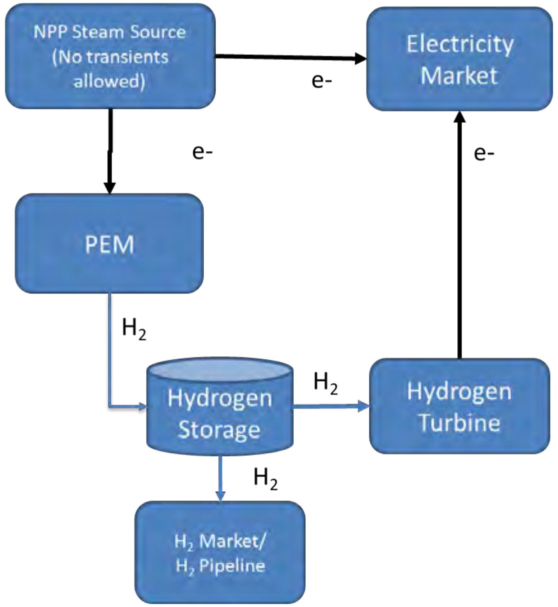
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

Hybrid Energy System Design Superstructures for Case Studies

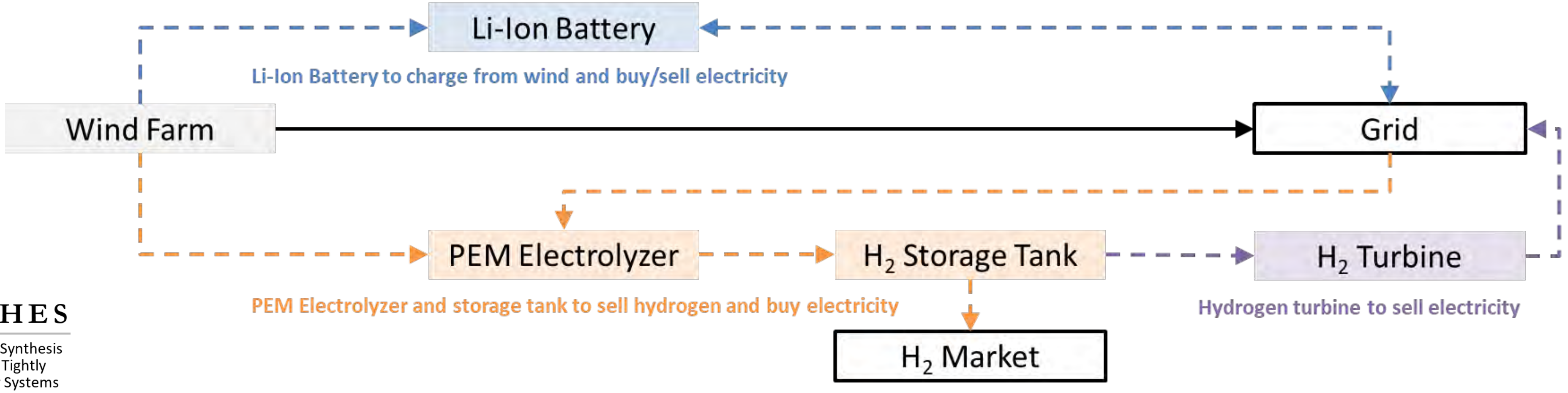
Advanced Fossil + Thermal Storage + Hydrogen + CCS



Nuclear + Hydrogen

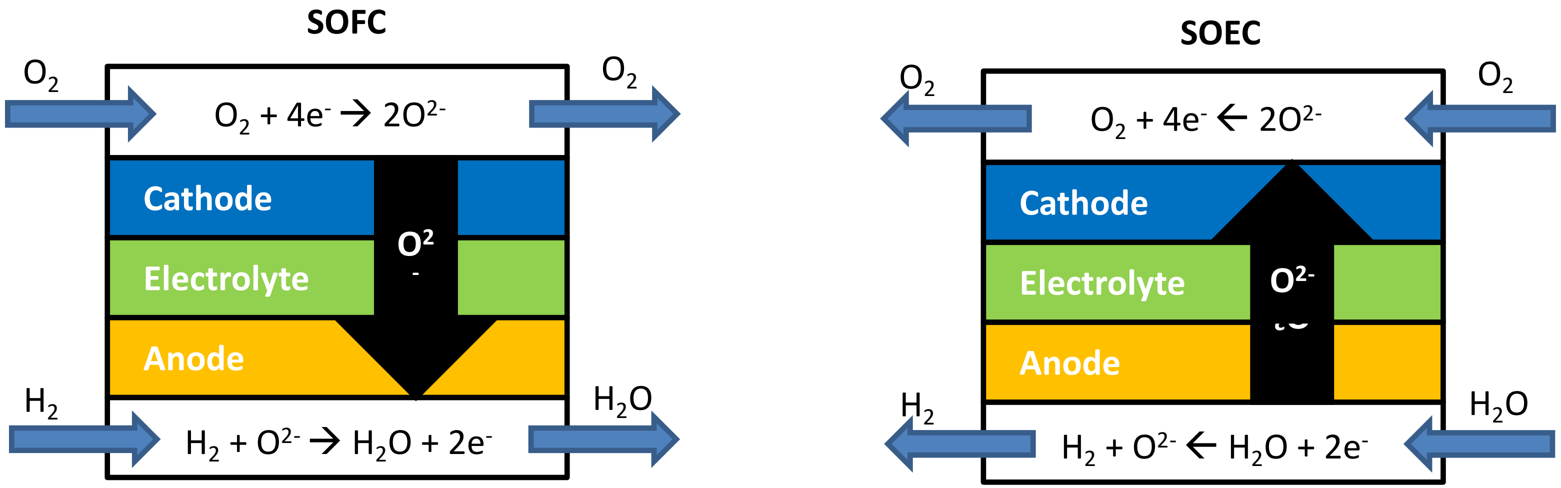


Renewables + Battery + Hydrogen



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

Integrated Energy Systems for H_2 Production & Use: SOFC/SOEC



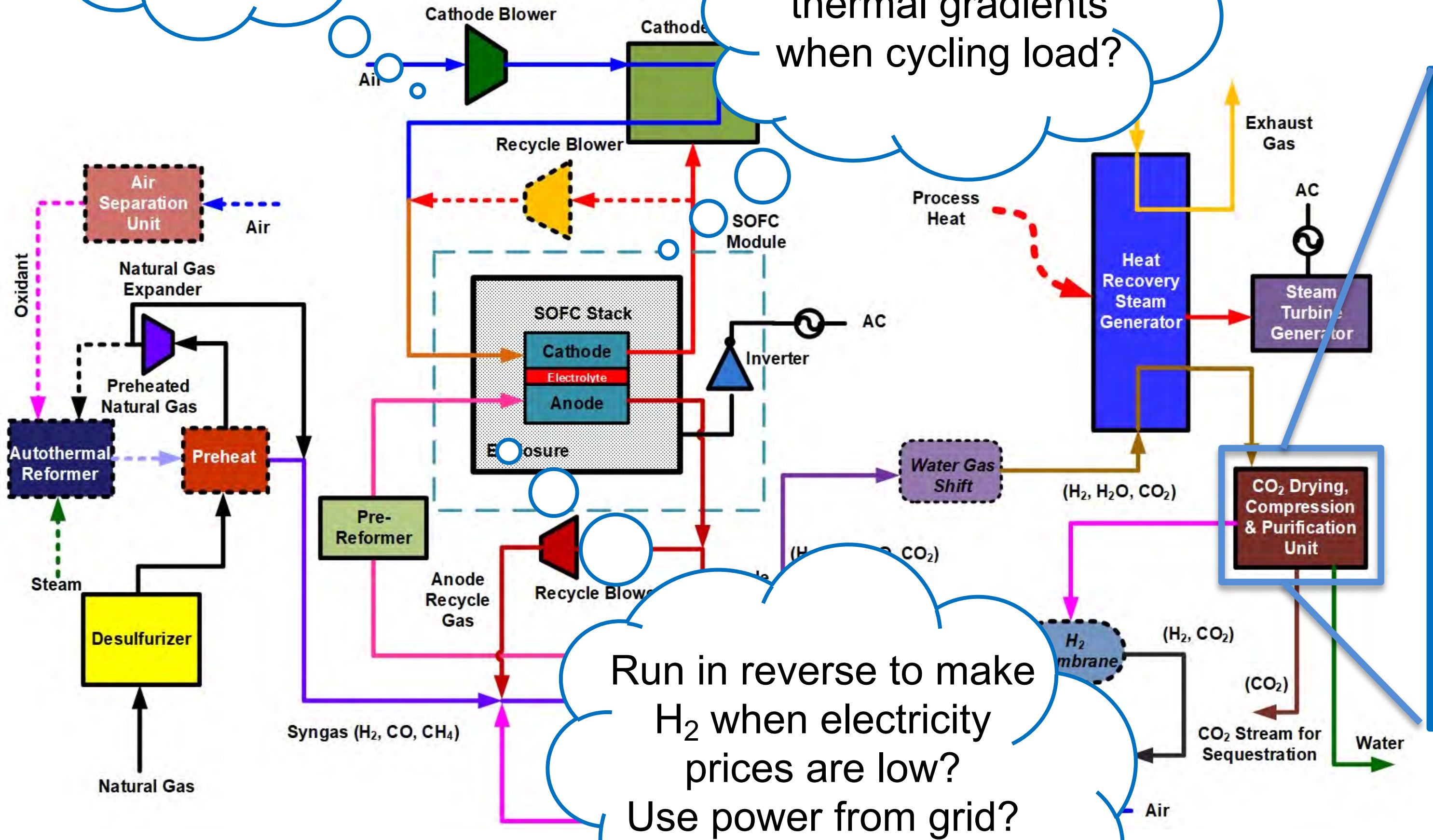
	HCC-SOFC Process Concepts	Scenario
1	SOFC + Gas Turbine + Steam Cycle + CCS	Variable Power
2	SOFC + Gas Turbine + Steam Cycle + Thermal Energy Storage + CCS	
3	NGCC + SOEC + CCS	Variable Power, Unlimited H_2 Demand
4	rSOFC + Gas Turbine + Steam Cycle + CCS	
5	SOFC + SOEC + Gas Turbine + Steam Cycle + CCS	
6	NGCC + SOEC + H_2 Storage/Turbine + CCS	Variable Power, Fixed or Limited H_2 Demand
7	rSOFC + Gas Turbine + Steam Cycle + H_2 Storage + CCS	
8	SOFC + SOEC + Gas Turbine + Steam Cycle + H_2 Storage + CCS	

Optimizing Operation of IES Process Designs

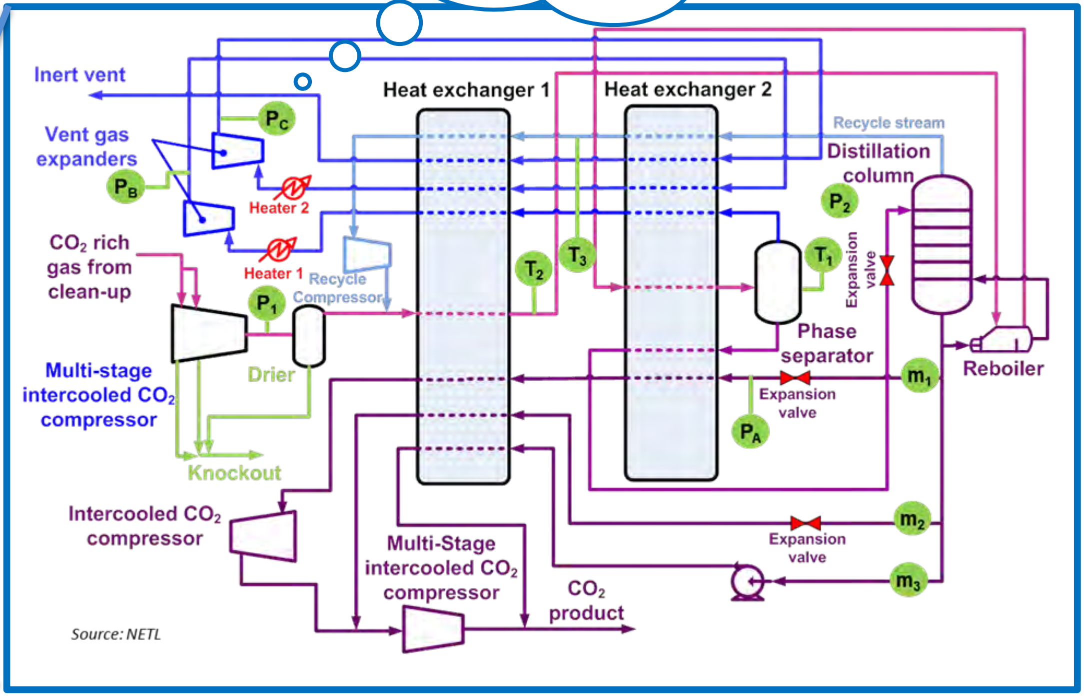
Operational limits of entire system?

How to manage thermal gradients when cycling load?

How can CPU meet specs across range of operation?



Run in reverse to make H_2 when electricity prices are low?
Use power from grid?
From storage?



CO_2 Compression & Purification Unit

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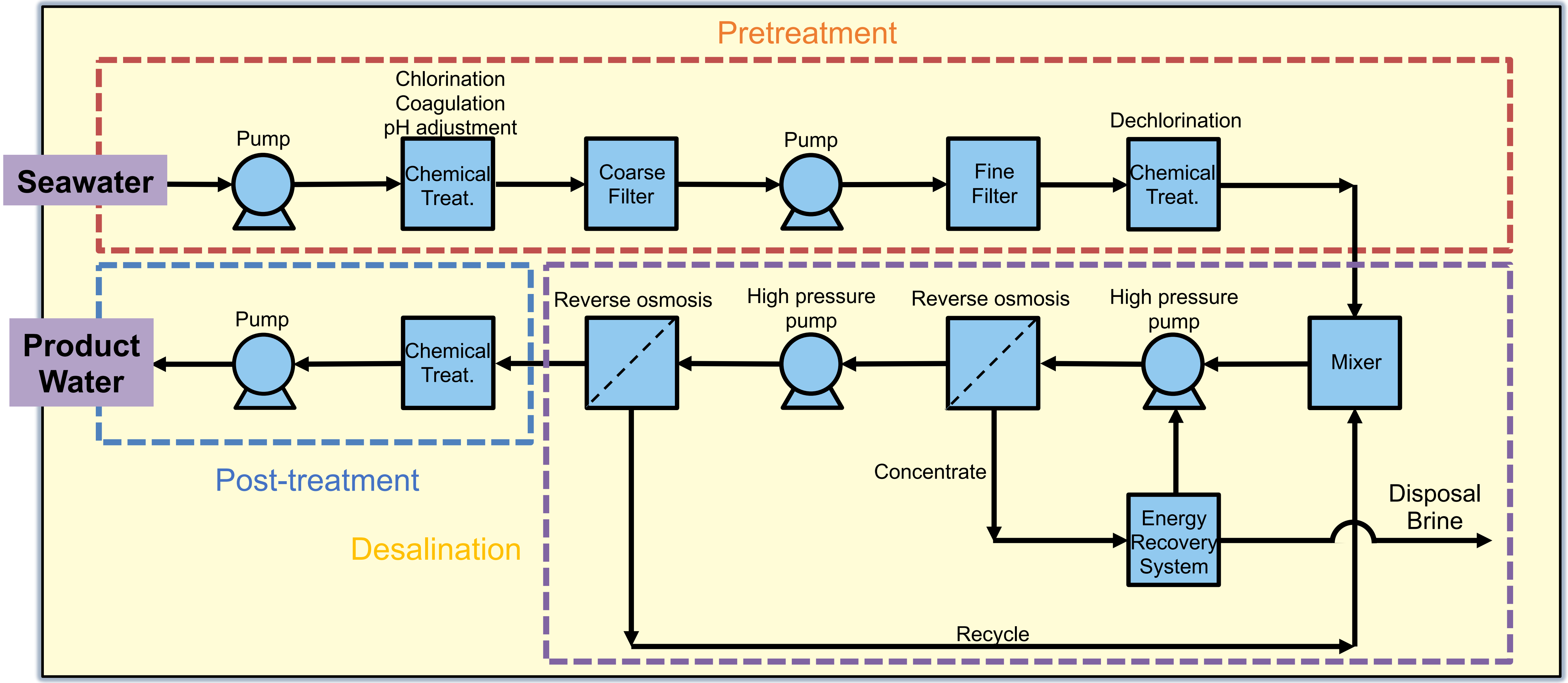
Water Desalination as Part of Integrated Energy Systems



Long Term Enterprise Expansion Planning Model

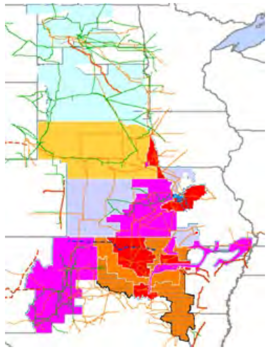
Development
- Open source – Requires commercial solver such as CPLEX
- Flexible
  - Modifications can address specific questions
  - Capture intermittency and volatility

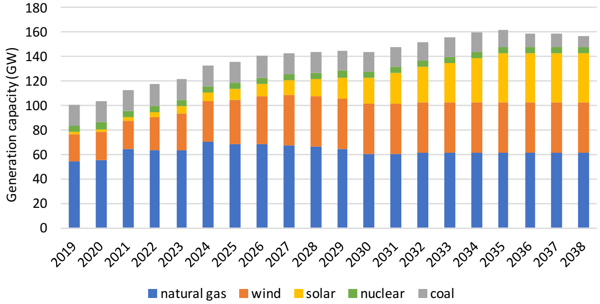
Timescales
- Yearly (decades) investment decision
- Hourly unit commitment problem

Inputs
- Aggerated spatial and temporal (representative days) information
- Operation and investment parameters, renewable capacity factor, load, etc.
- Existing transmission between regions

Outputs
- Location, year, type and number of generators, transmission lines and storage units to install
- When to retire or extend life
- Transmission expansion between regions
- Approximate operating schedule

Limitations
- Limited to 1 hour time intervals (some extreme ramp rate scenarios not accounted for)
- Number of representative days and balancing regions limited due to trackability
- Data can be time consuming to aggerate for specific regions (ERCOT and SPP currently modeled)





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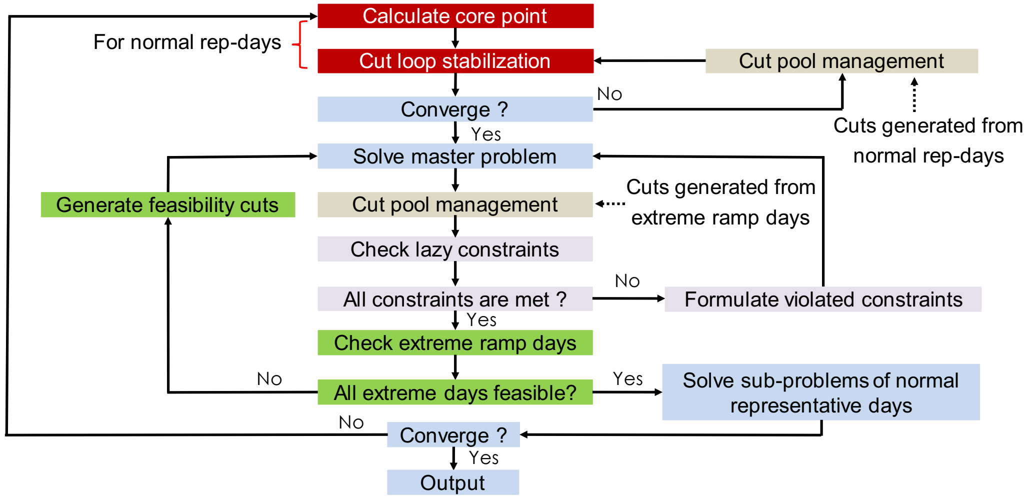
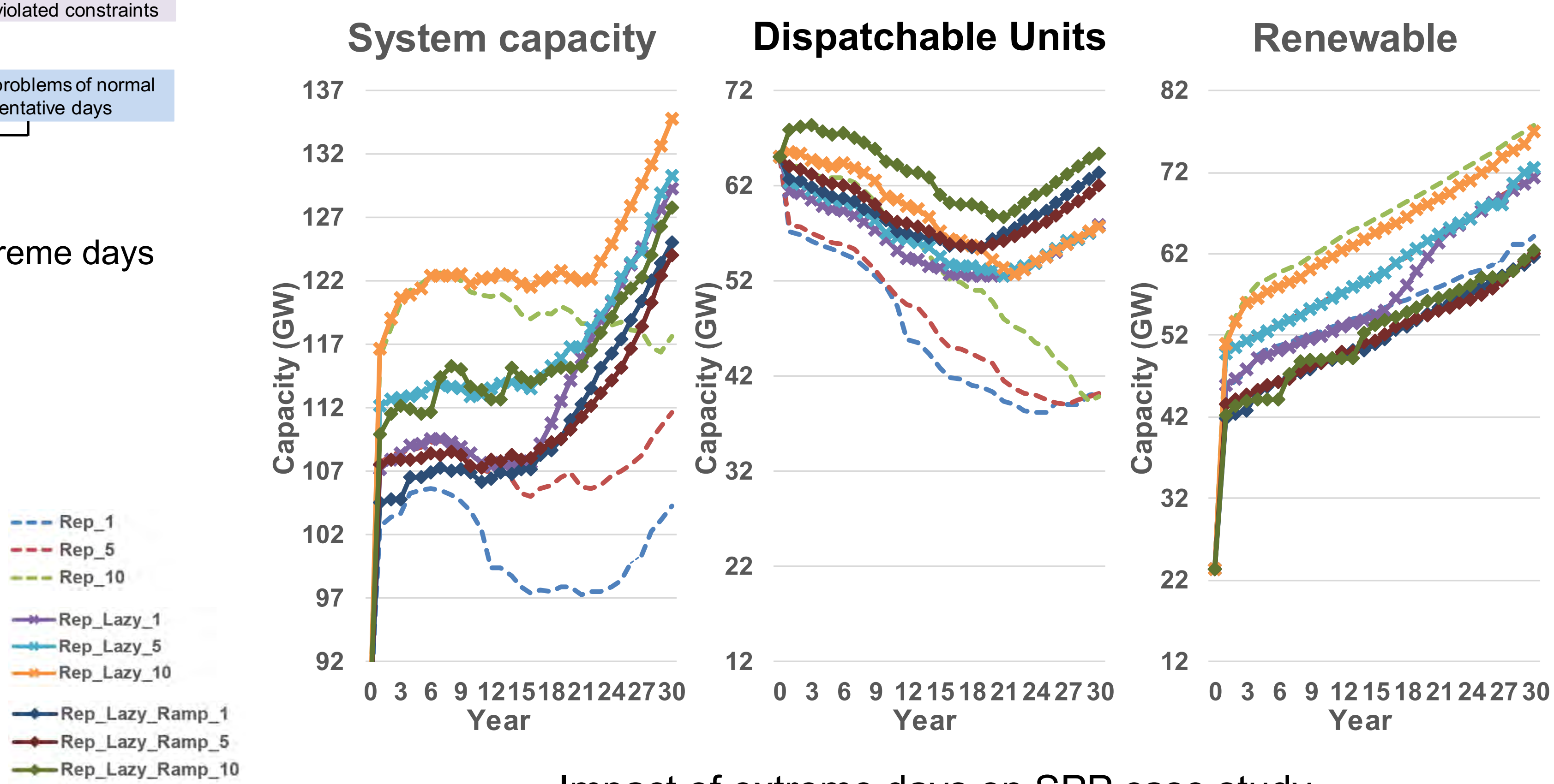
Lara, C. L., Siirola, J. D., & Grossmann, I. E. (2019). Electric power infrastructure planning under uncertainty: stochastic dual dynamic integer programming (SDDiP) and parallelization scheme. Optimization and Engineering, 1-39. Lara, C. L., Mallapragada, D. S., Papageorgiou, D. J., Venkatesh, A., & Grossmann, I. E. (2018). Deterministic electric power infrastructure planning: Mixed-integer programming model and nested decomposition algorithm. European Journal of Operational Research, 271(3), 1037-1054.

Identifying Opportunities for Future Integrated Energy Systems



Cut generation algorithm for incorporating extreme days



Impact of extreme days on SPP case study

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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

Partnership and Impact

Stakeholder Advisory Board

- Keep informed of developments, progress
- Provide input on key challenges

Collaborate with IDAES to apply the tools

- Cooperative Research & Development Agreement (CRADA)
  - Protects IP, enables information sharing

Join the IDAES development community (Open Source Release Available)

- Access to IDAES Integrated Platform
- Opportunity to expand capabilities of the tools

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Acknowledge support from the U.S. Department of Energy, Office of Fossil Energy, through the Simulation-Based Engineering/Crosscutting Research Program

National Energy Technology Laboratory: David Miller, Tony Burgard, John Eslick, Andrew Lee, Miguel Zamarripa, Jinliang Ma, Dale Keairns, Jaffer Ghouse, Ben Omell, Chinedu Okoli, Richard Newby, Maojian Wang
Sandia National Laboratories: John Siirola, Bethany Nicholson, Carl Laird, Katherine Klise, Dena Vigil, Michael Bynum, Ben Knueven
Lawrence Berkeley National Laboratory: Deb Agarwal, Dan Gunter, Keith Beattie, John Shinn, Hamdy Elgammal, Joshua Boverhof, Karen Whitenack, Oluwamayowa Amusat
Carnegie Mellon University: Larry Biegler, Nick Sahinidis, Chrysanthos Gounaris, Ignacio Grossmann, Owais Sarwar, Natalie Isenberg, Chris Hanselman, Marissa Engle, Qi Chen, Cristiana Lara, Robert Parker, Ben Sauk, Vibhav Dabadghao, Can Li, David Molina Thierry
West Virginia University: Debangsu Bhattacharyya, Paul Akula, Anca Ostace, Quang-Minh Le
University of Notre Dame: Alexander Dowling, Xian Gao

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

National Energy Technology Laboratory: David Miller, Andrew Lee, Jaffer Ghouse
Sandia National Laboratories: John Siirola, Michael Bynum
Idaho National Laboratory: Cristian Rabiti, Andrea Alfonsi, Konor Frick
National Renewable Energy Laboratory: Wes Jones, Darice Guittet, Jordan Jalving, Ben Kneuven
Lawrence Berkeley National Laboratory: Dan Gunter, Keith Beattie
University of Notre Dame: Alexander Dowling, Xian Gao

GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

We also acknowledge support from AMO/NAWI and ARPA-E for IDAES-related efforts discussed in this presentation

NAWI National Alliance for Water Innovation

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