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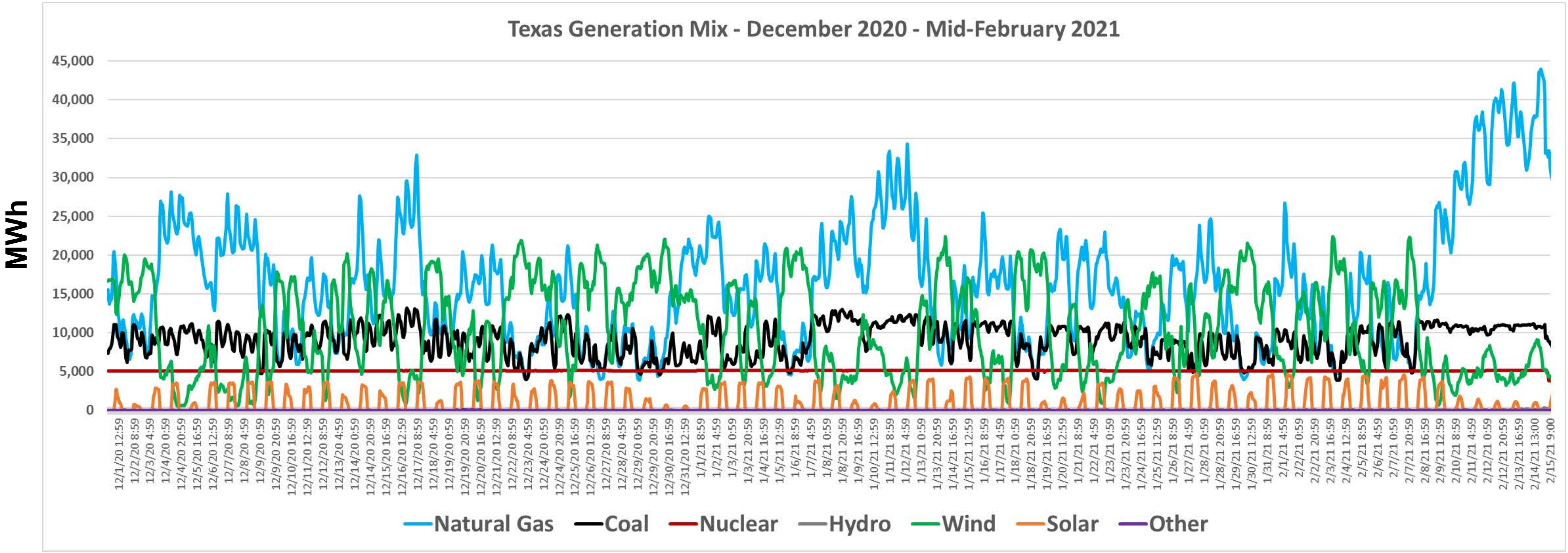
David C. Miller, Ph.D.

Senior Fellow

National Energy Technology Laboratory

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

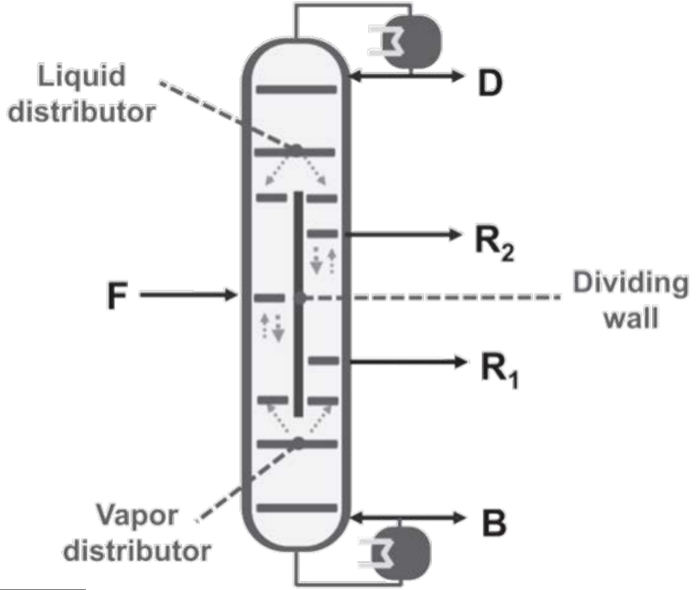
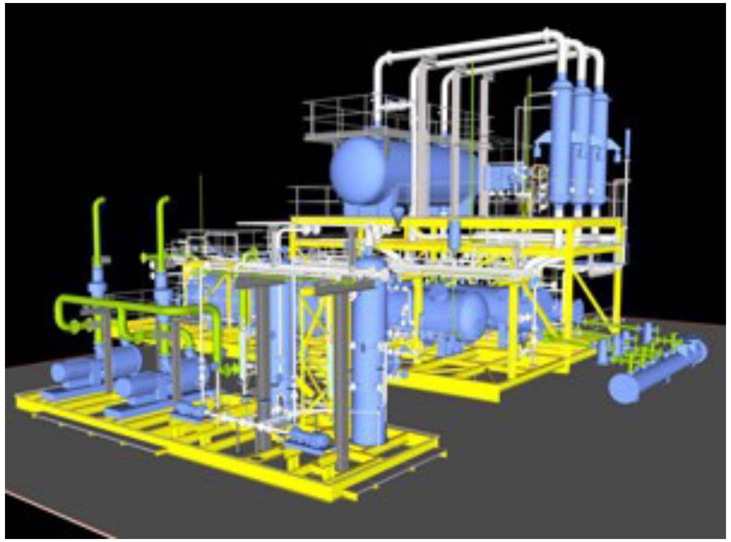


Figure from Rawlings et al., 2019



RAPID Transforming Process Industries

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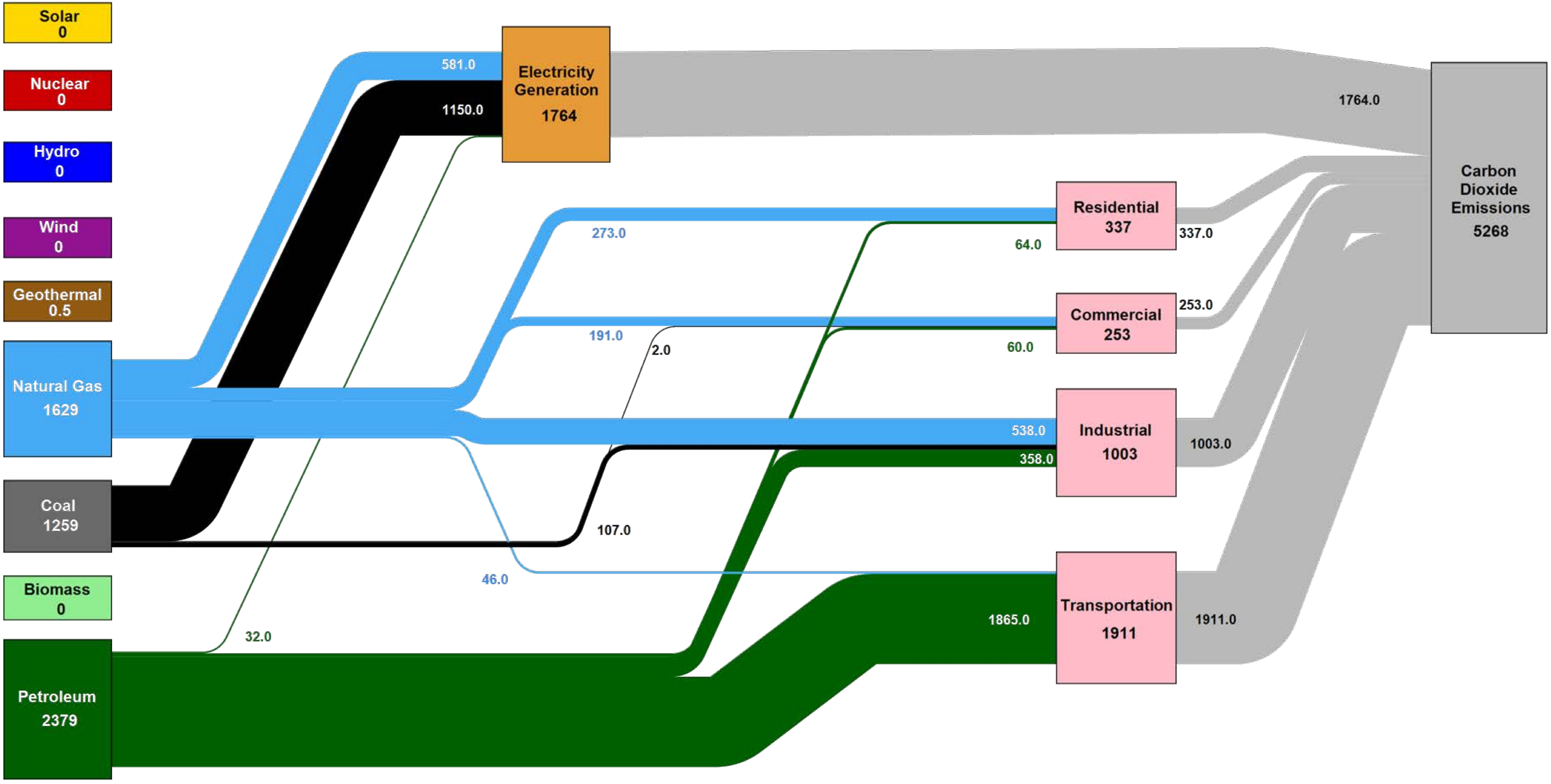
Estimated U.S. Carbon Dioxide Emissions in 2018: ~5,268 Million Metric Tons

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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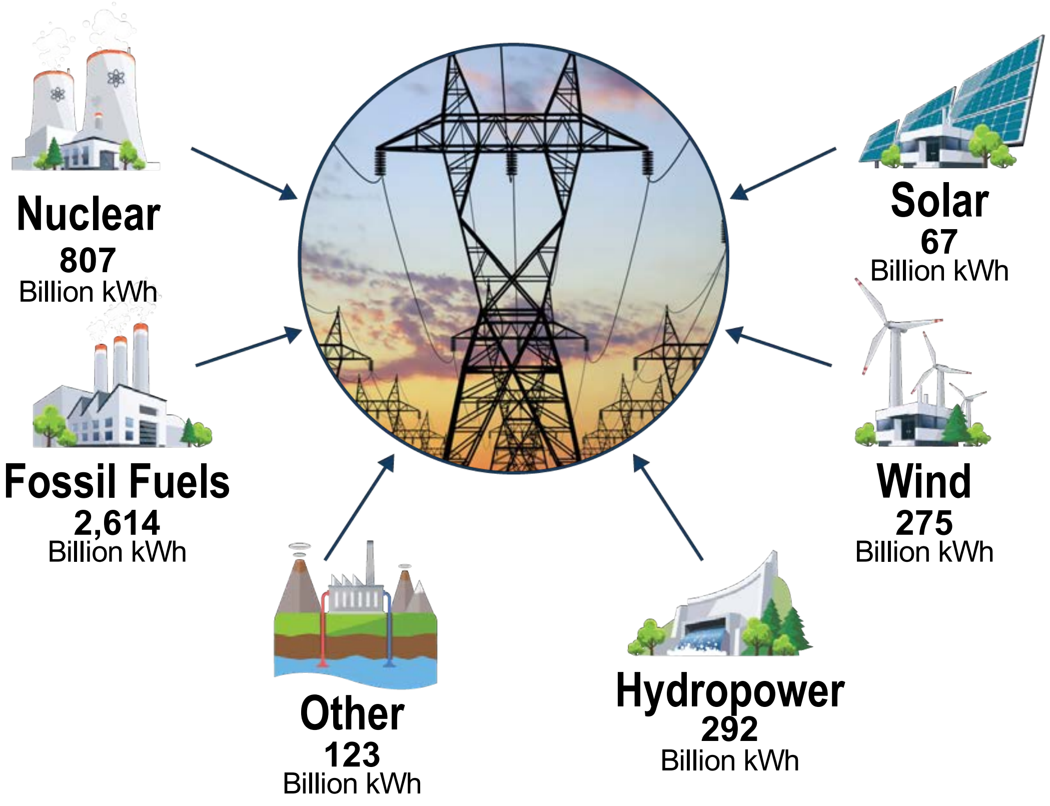
Integrated Energy Systems Expand Design Space

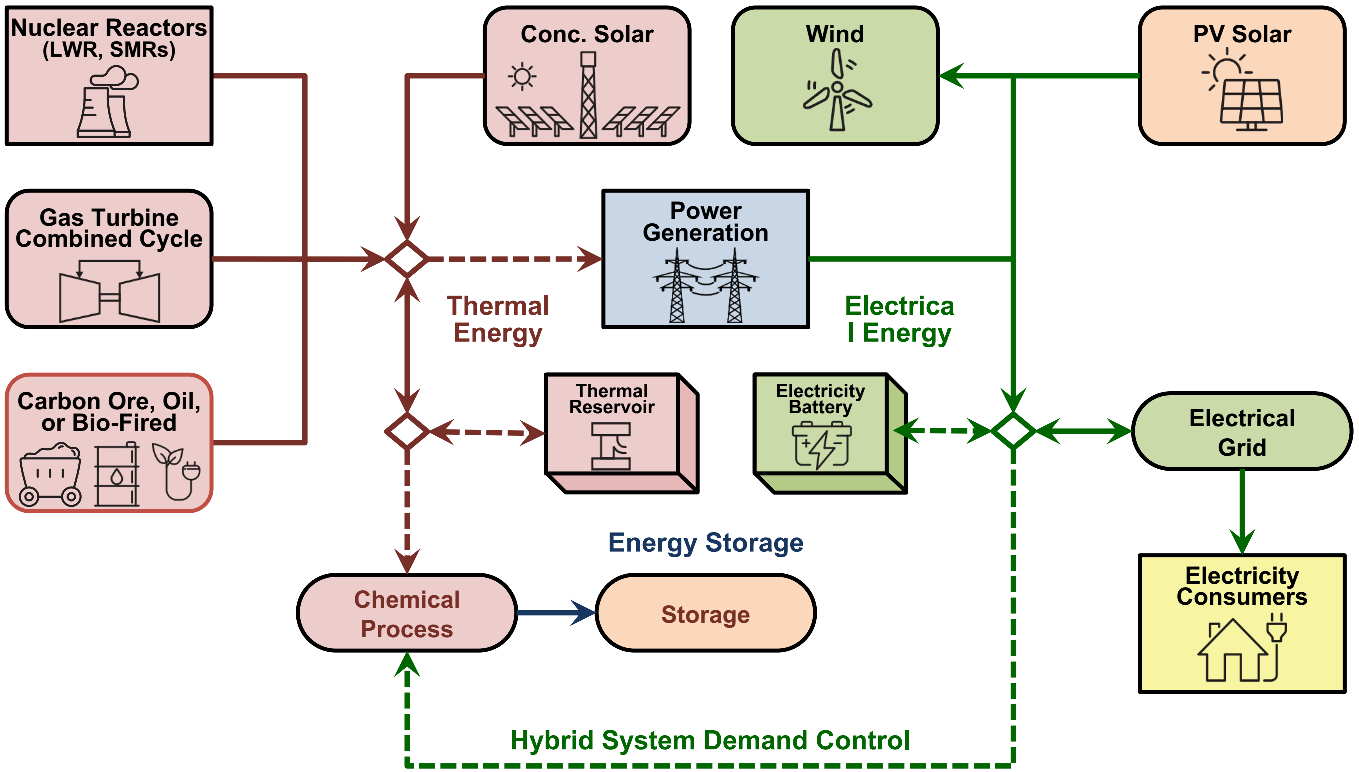
Coordinated Energy Systems



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

Data source: EIA, 2018

Integrated Energy Systems



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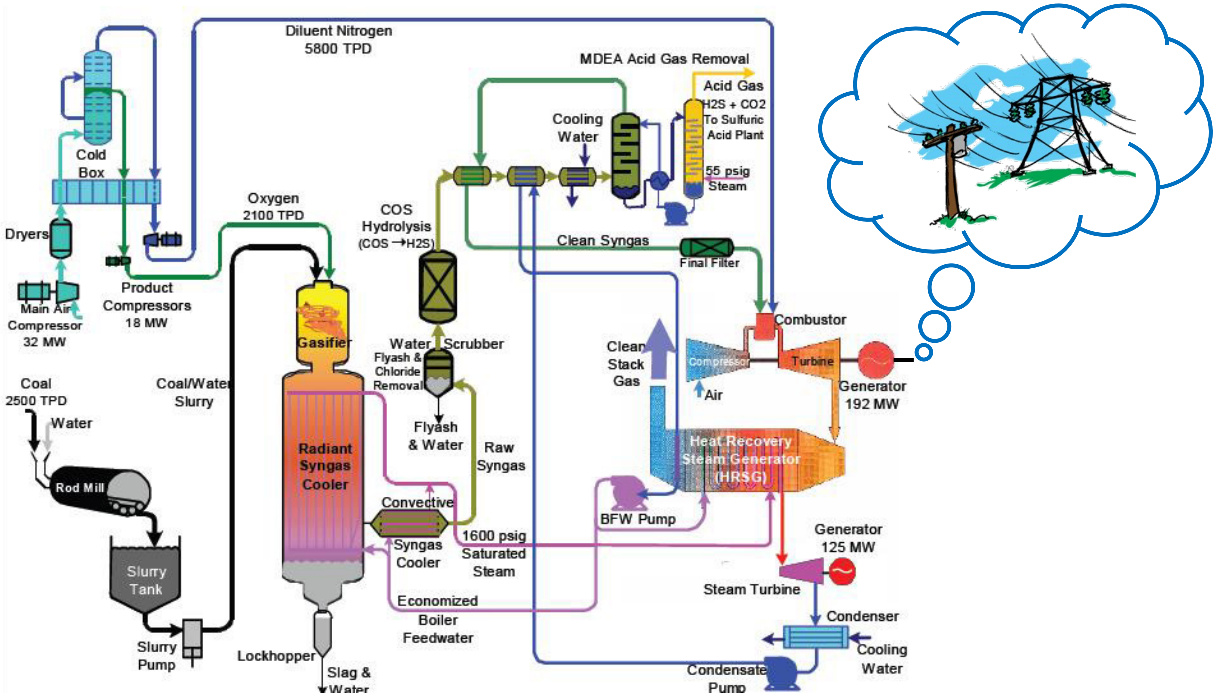
Energy System Analysis is Often Applied in Isolation

Process-centric Modeling

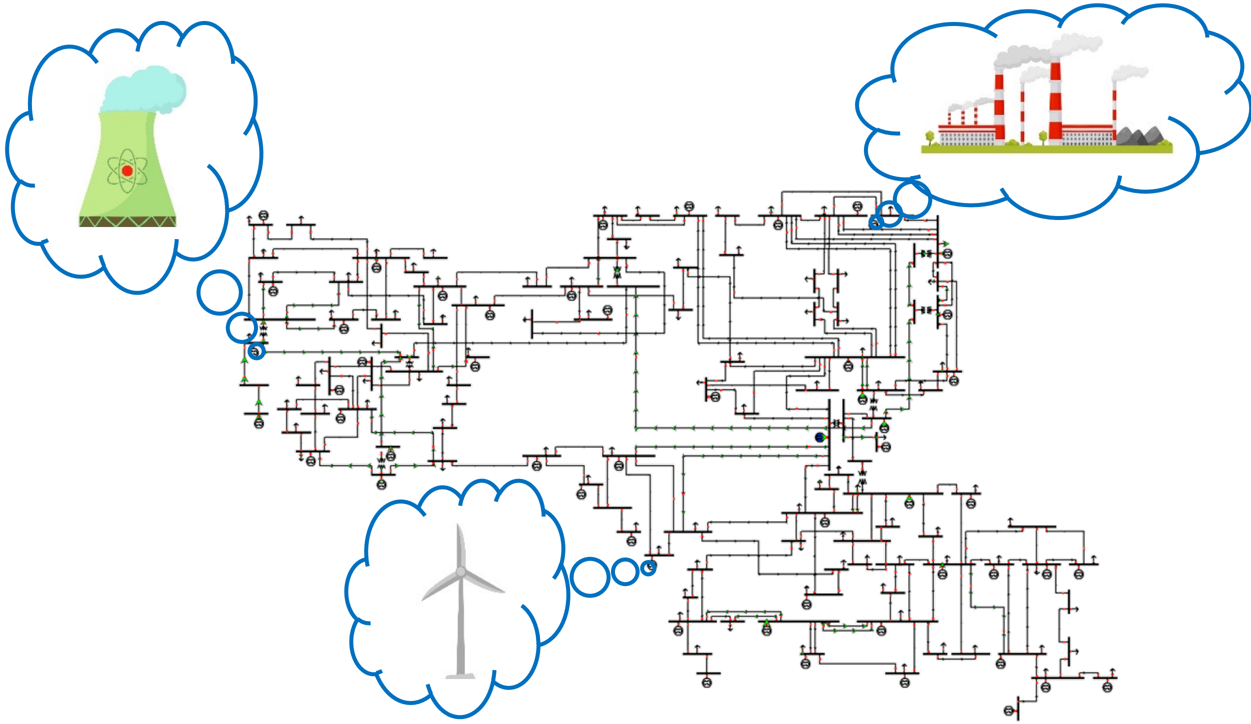
Detailed steady state or dynamic process models,
with the grid modeled as an infinite capacity bus



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

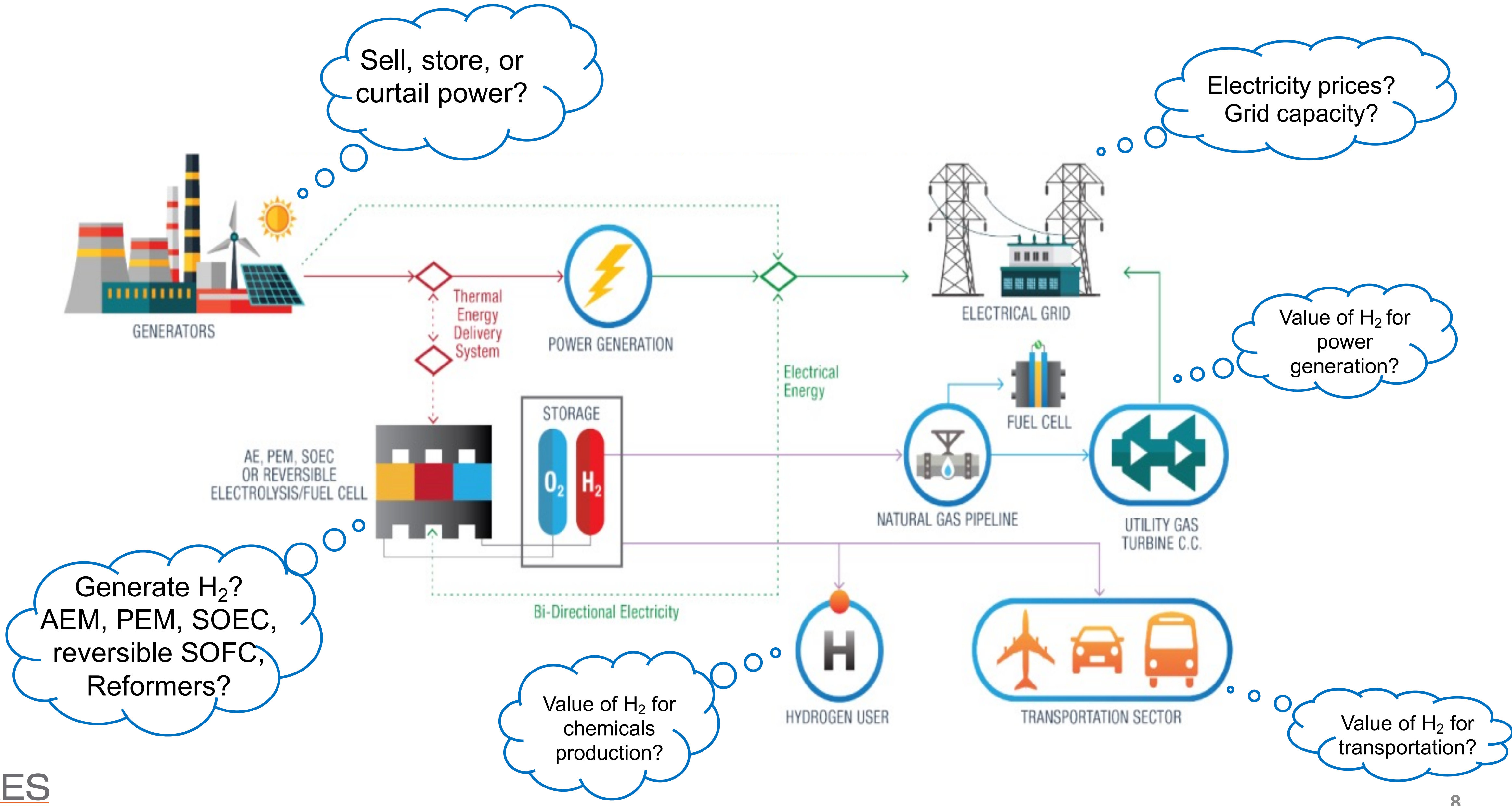
Grid-centric Modeling

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

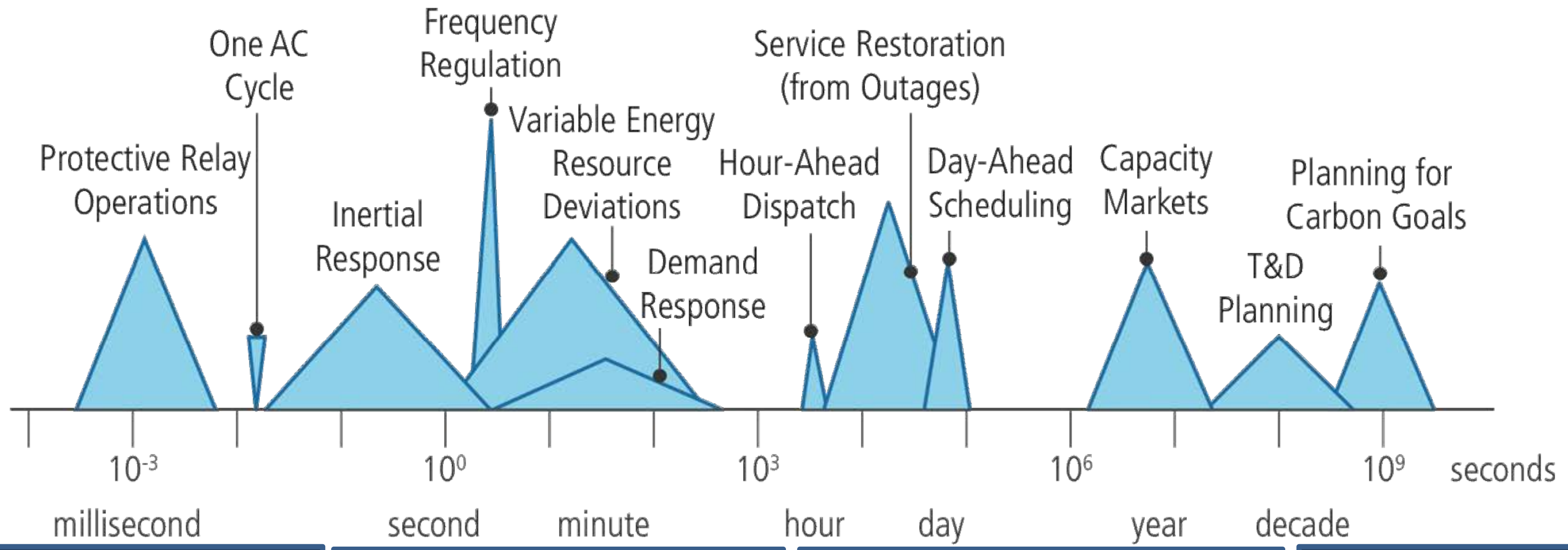


https://icseg.iti.illinois.edu/files/2013/10/IEEE118.png

Integrated Energy System For Power and H_2 Production



Multiple Time Scales & Perspectives Across Tools



Real-Time Operations

High frequency dynamics

Electricity Grid
Dispatch, Power Flow

Complex effects of new generators

Capacity Expansion
20-30 Year Horizon

Difficult to value flexibility, reliability

Energy Economy Models

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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Trends Requiring Innovation in Decision Support Tools

- Evolving energy ecosystem requires greater flexibility
- Expanding U.S. industry
- Process intensification & modularization
- 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

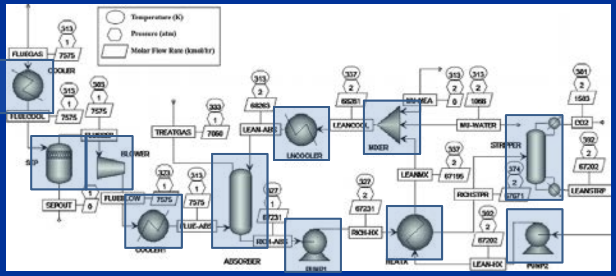
Understanding large, complex systems: Don’t Simulate → Solve

Optimization over degrees of freedom only

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

u ↓ ↑ f

Simulator



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

Optimization with embedded algebraic model as constraints

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

Glass-box optimization
~ 1-5 STE

[Adapted from Biegler, 2017]

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IDAES Integrated Platform

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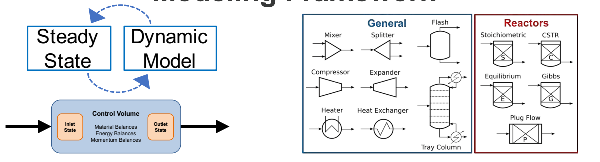
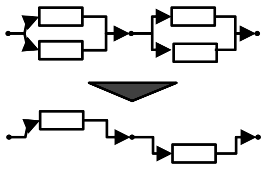
Modeling Framework

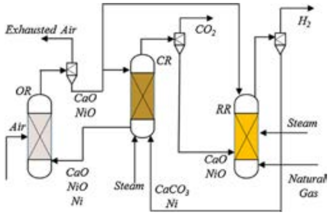


Hierarchical - Steady-State & Dynamic - Model Libraries

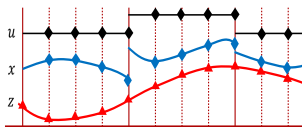
Conceptual Design	Plant Design Process Optimization	Process Operations Dynamics & Control	Uncertainty Quantification Robust Optimization	AI/ML Surrogate Modeling	Enterprise Optimization Grid & Planning	Materials Optimization

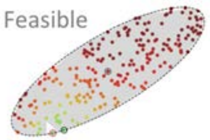


PYOMO GDP



caprese

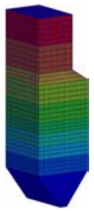




PyROS

ALAMO a black-box modeling tool

PySMO



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

Recent Applications, Impact, and Extensions

Design space exploration: Reduced energy demand by >40% through automated exploration of 42 million alternatives

Process Improvements: Improved minimum operating load by 44% and increased overall efficiency

Bridging timescales: Captures complex interactions among generators & bulk power market to enable analysis of emerging flexible energy systems with energy storage

NAWI National Alliance for Water Innovation — IDAES is the platform for ProteusLib, a comprehensive water treatment modeling library being developed under the AMO Water Hub

DISPATCHES Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems — IDAES is the platform for the GMLC DISPATCHES project to develop and demonstrate an open, transparent, multi-lab computational platform to support the design, optimization, and analysis of tightly coupled hybrid systems with zero or negative CO_2 emissions. Industry partners: NRECA, Exelon, Storworks, ACES

GRID MODERNIZATION LABORATORY CONSORTIUM U.S. Department of Energy

arpa-e CHANGING WHAT'S POSSIBLE — IDAES is being applied to the design and optimization of Flexible Carbon Capture Systems under the ARPA-E FLECCS Program in conjunction with industry partners (Susteon (Lead), Svante, LADWP, SoCalGas/Sempra Energy).

CRADA Cooperative Research & Development Agreement — IDAES is exploring the design space to optimize Direct Air Capture (DAC) under a CRADA with industry partner ExxonMobil Research.

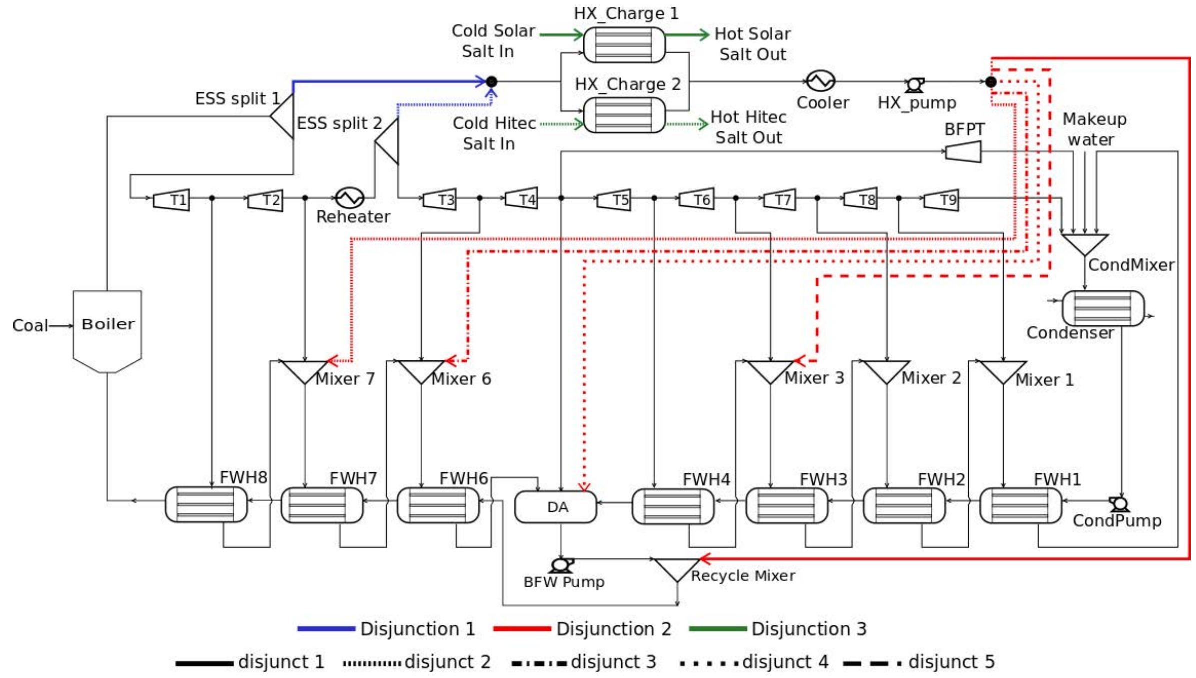
SBIR — IDAES is the foundation for SBIR Projects with 6 companies

Terrafore Technologies LLC · MICROBEAM TECHNOLOGIES, INC. · MapEx · Aerem Nova Energy Storage · Envergex Sparking Innovations · CRAFT Tech Combustion Research and Flow Technology, Inc.

Conceptual Design of Thermal Energy Storage with GDP

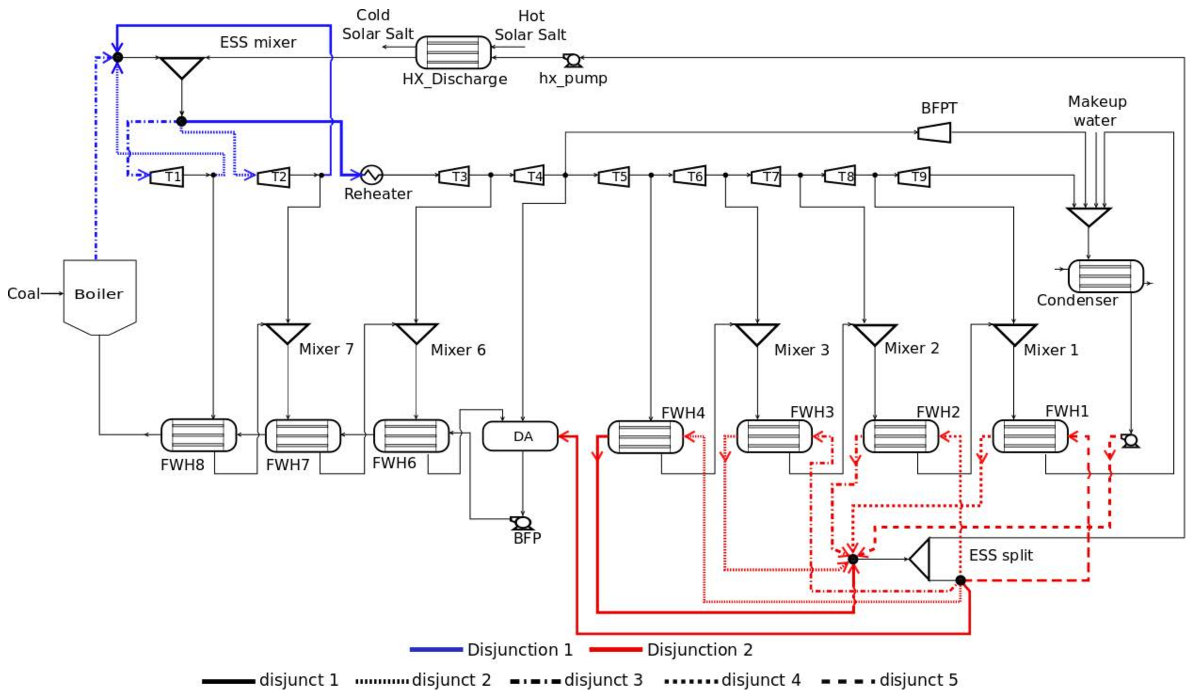
Charging Case (20 possibilities)

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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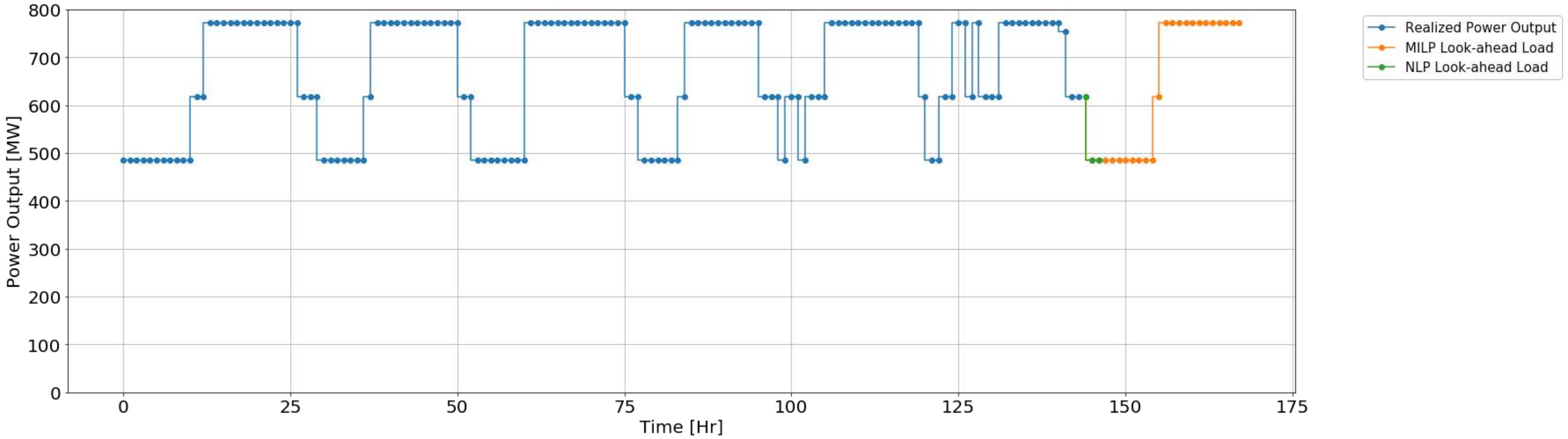
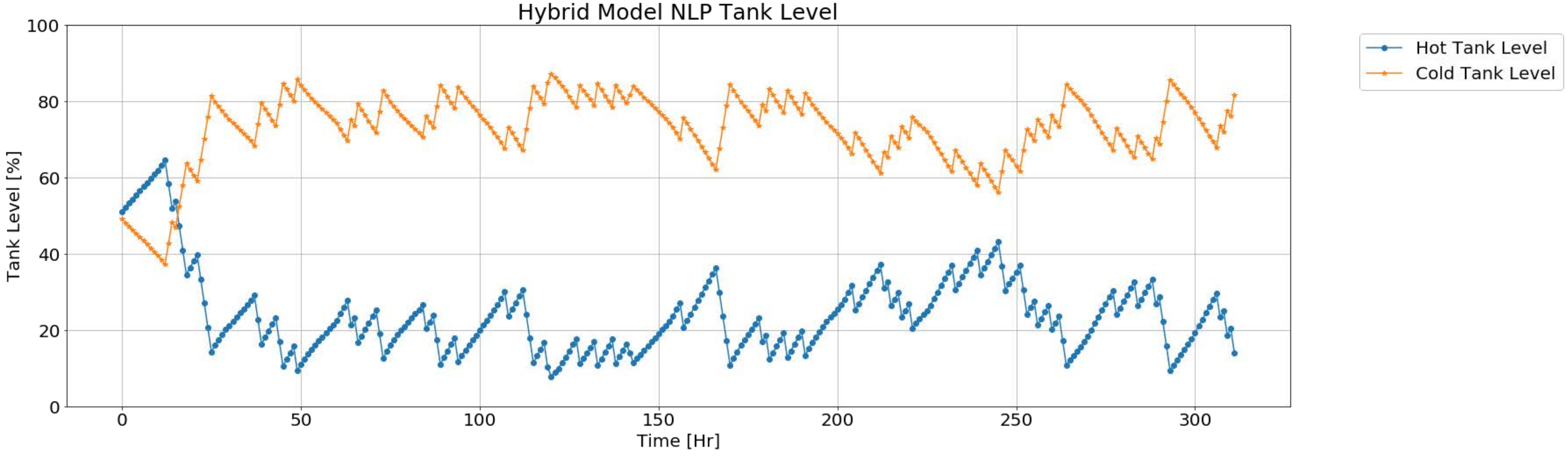
NMPC Control of Generator + Thermal Energy Storage

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





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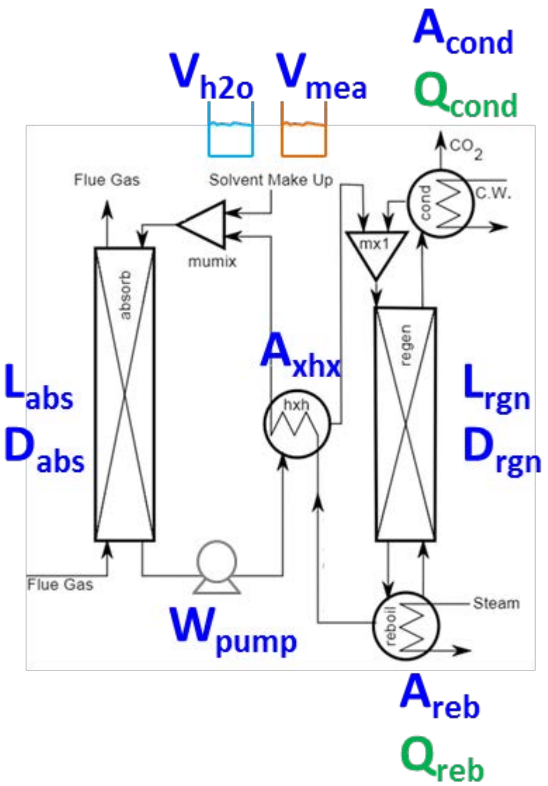
Robust Design to Reduce Technical Risk

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

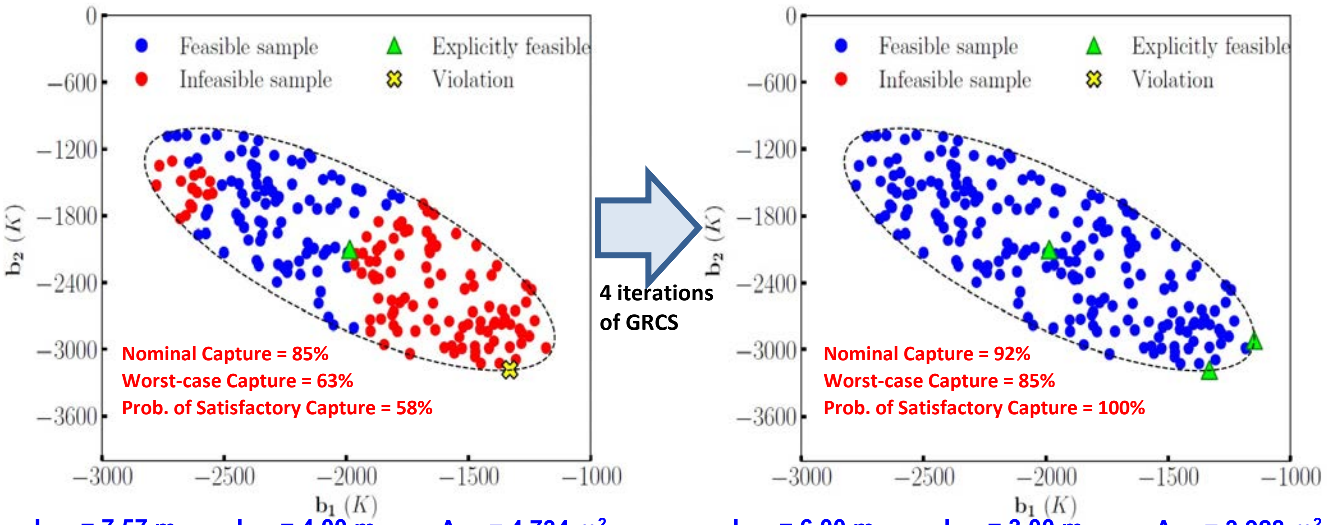


Deterministic Solution

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

Robust Solution

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



Deterministic solution:

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 solution:

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*

Long Term Enterprise Expansion Planning Model

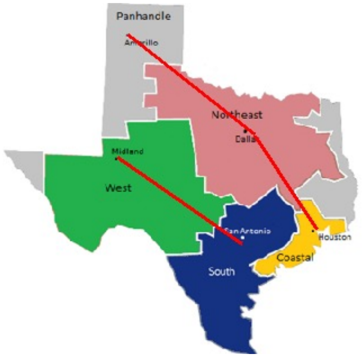
Development
- Open source – Requires commercial solver such as CPLEX
- Flexible
  - Modifications can address specific questions
  - Capture intermittency and volatility

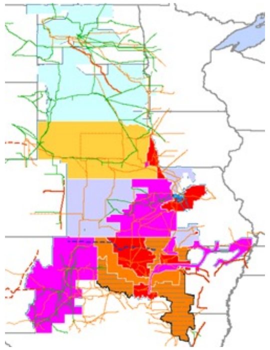
Timescales
- Yearly (decades) investment decision
- Hourly unit commitment problem

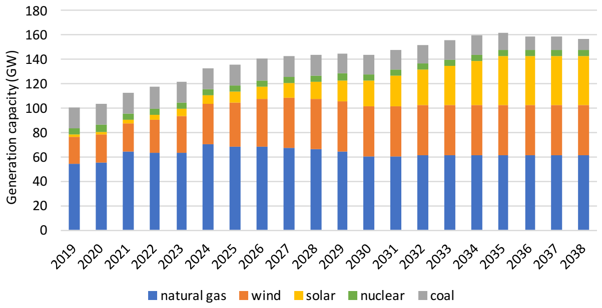
Inputs
- Aggerated spatial and temporal (representative days) information
- Operation and investment parameters, renewable capacity factor, load, etc.
- Existing transmission between regions

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)

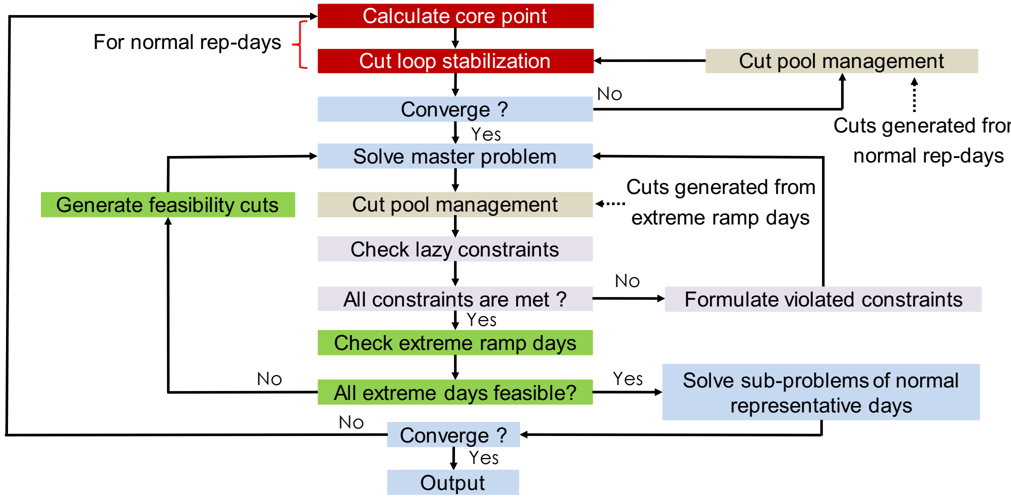




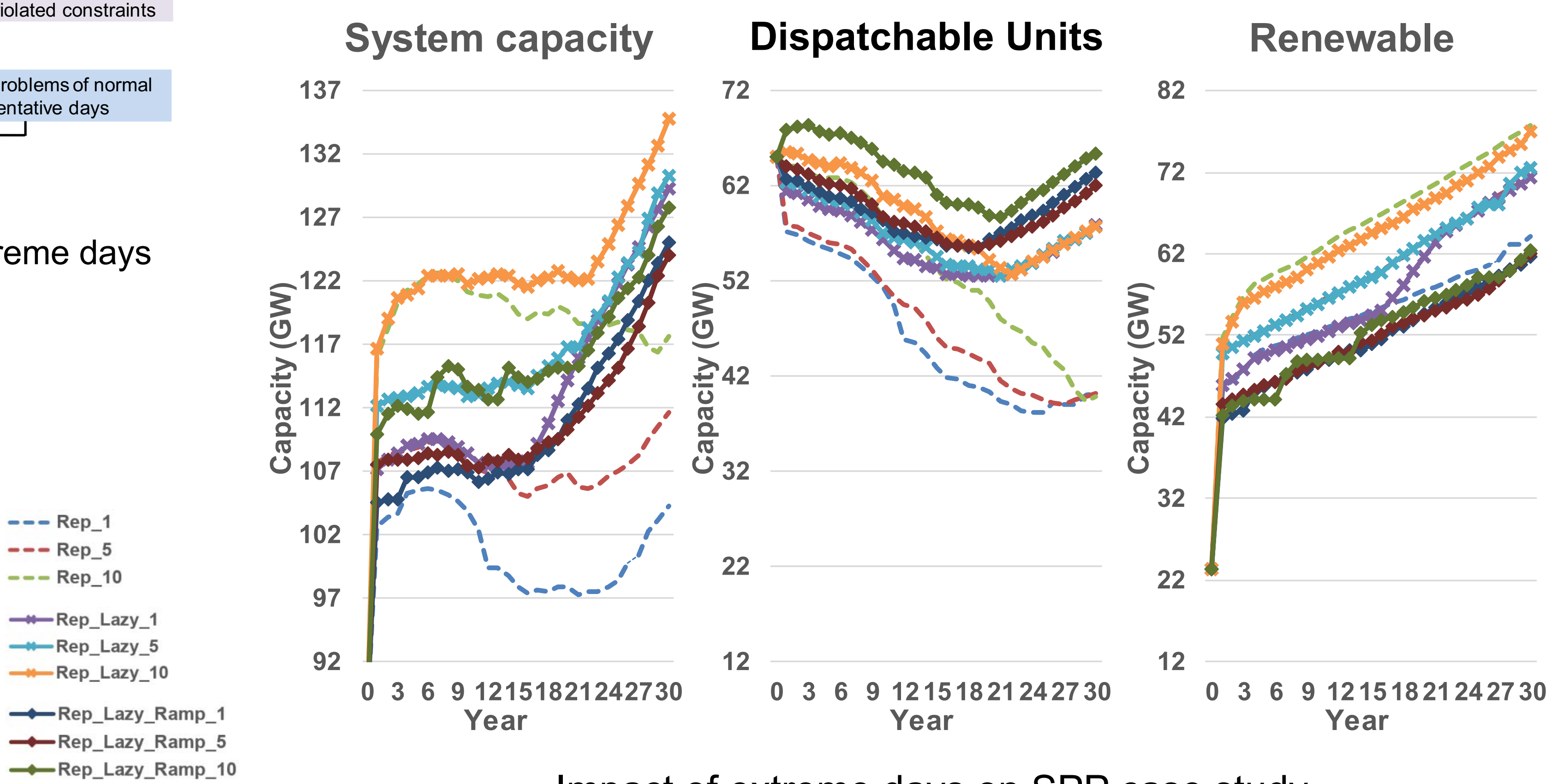


Lara, C. L., Siirola, J. D., & Grossmann, I. E. (2019). Electric power infrastructure planning under uncertainty: stochastic dual dynamic integer programming (SDDiP) and parallelization scheme. Optimization and Engineering, 1-39. Lara, C. L., Mallapragada, D. S., Papageorgiou, D. J., Venkatesh, A., & 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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Components of IDAES in 2021

- **IDAES-Core** (Simulation-Based Engineering/Crosscutting Program)
  - Stakeholder & Program Support
  - Software Development and Release Management; Standardization and Verification; Platform Integration; Interfaces and Usability
  - Machine Learning and Artificial Intelligence
  - Dynamic Modeling Infrastructure Development
  - Uncertainty Mitigation
- **IDAES-IES** (FE Crosscutting) - Focus on unique needs for IES
  - Design of Flexible Dynamic Energy Systems
  - Dynamic Grid/Market Interactions
  - Dynamic Distribution Networks for IES
- **SOFC-IES** (FE SOFC/IES Program)
  - Evaluation of SOEC/SOFC Integrated Energy Systems
  - Dynamics and Control of Flexible Integrated Energy Systems
- **TTNEP** (FE TPG Program) - IES for Power and Blue Hydrogen Co-Production

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

idaes.org

github.com/IDAES/idaes-pse

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The IDAES Technical Team:

- **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
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- **West Virginia University**: Debangsu Bhattacharyya, Paul Akula, Anca Ostace, Quang-Minh Le
- **University of Notre Dame**: Alexander Dowling, Xian Gao