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Generalized Disjunctive Programming in IDAES Framework:

Conceptual Design of Ultra-supercritical Power Plant Integrated with Thermal Energy Storage

Edna Soraya Rawlings, Naresh Susarla, Jaffer Ghouse, John Siirola, and David Miller

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INFORMS 2022

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IDAES Integrated Platform

Institute for the Design of Advanced Energy Systems

GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

Team

Sandia National Laboratories · National Energy Technology Laboratory · Berkeley Lab · Carnegie Mellon · Georgia Tech · West Virginia University · University of Notre Dame

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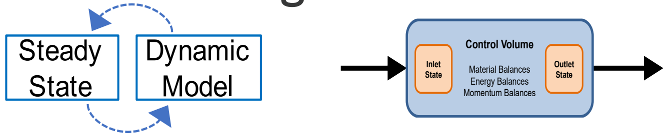
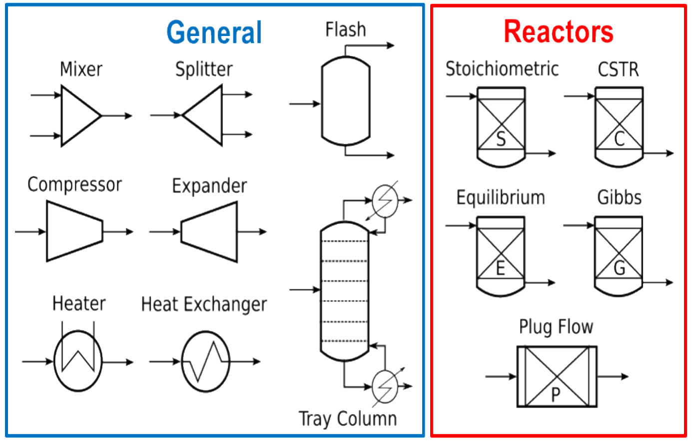
Georgia Institute of Technology: Nick Sahinidis

IDAES team at the IDAES meeting in February, 2020.

Modeling Framework



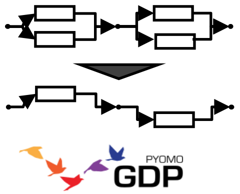


- ✓ Hierarchical - Steady-State and Dynamic - Model Libraries
- ✓ Open Source:

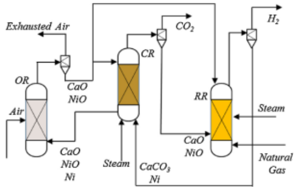
https://github.com/IDAES/idaes-pse

Capabilities

Conceptual Design



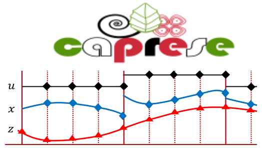
Plant Design Process Optimization



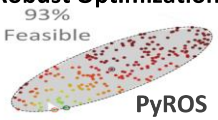
AI/ML Surrogate Modeling

ALAMO · PySMO

Process Operations Dynamics & Control



Uncertainty Quantification Robust Optimization



Enterprise Optimization Grid & Planning

- ✓ Supports the design, optimization, and analysis of tightly coupled hybrid energy systems
- ✓ Library of integrated energy system models:

https://github.com/gmlc-dispatches/dispatches

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

PYOMO

python™

Gurobi	CPLEX	Xpress	CBC	Ipopt
GAMS	NEOS	Mosek	BARON	GLPK

DISPATCHES Team

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

National Energy Technology Laboratory: David Miller, Andrew Lee, Jaffer Ghouse, Andres Calderon, Naresh Susarla, Radhakrishna Gooty

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Lawrence Berkeley National Laboratory: Dan Gunter, Keith Beattie, Oluwamayowa Amusat

University of Notre Dame: Alexander Dowling, Xian Gao, Xinhe Chen

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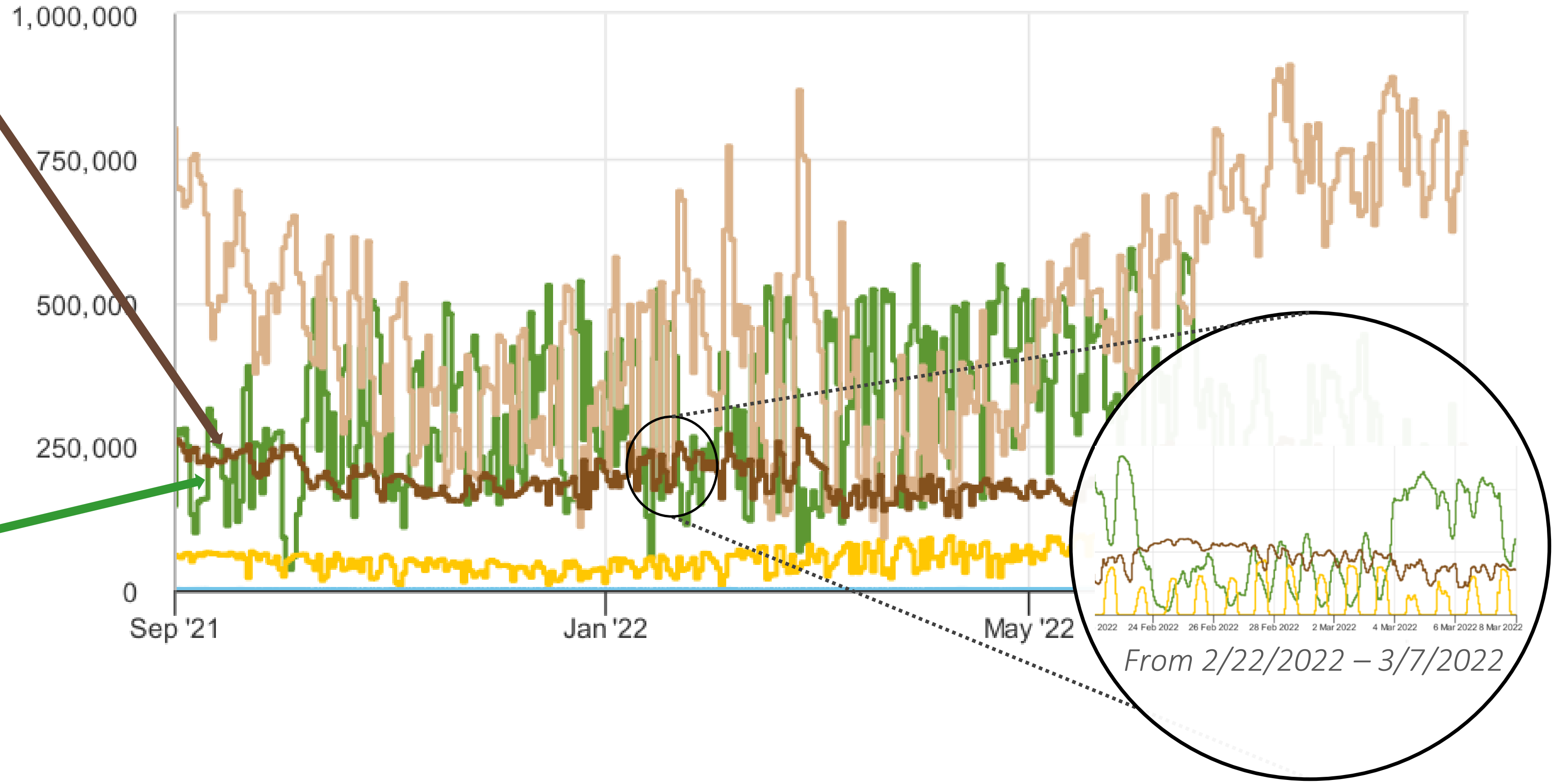
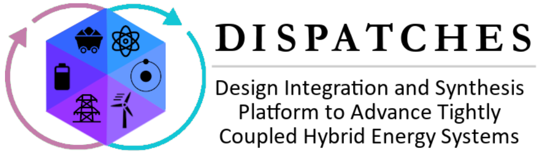
Motivation: Introduction of renewable electricity requires flexibility

Coal plants in the U.S.[1]

Natural gas, solar, and wind plants in the U.S.[1]

Electric Reliability Council of Texas, Inc. (ERCO) electricity generation by energy source 9/1/2021 – 9/1/2022, Eastern Time[2]

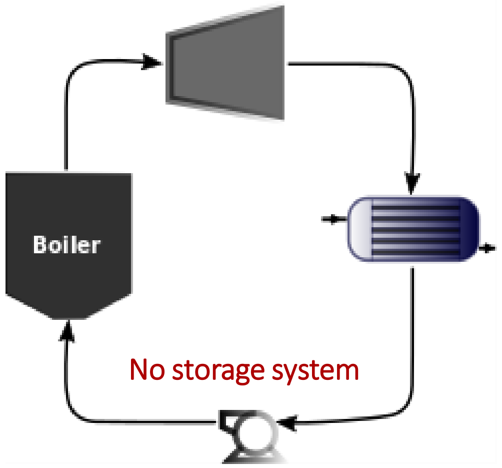




[1] Source: U.S. Energy Information Administration. U.S. Energy Mapping System, https://www.eia.gov/state/maps.php. Accessed July 2, 2021. [2] Source: U.S. Energy Information Administration. Hourly Electric Grid Monitor, https://www.eia.gov/electricity/gridmonitor/expanded-view/custom/pending/GenerationByEnergySource-4/edit, Accessed September, 2022

Optimization-based conceptual design of energy systems

- **Opportunity:**
  - Integrate existing energy systems with thermal energy storage (TES)
  - Charge and discharge storage operating cycles



Rankine Cycle
Heating
Expansion
Condensation
Pumping

Power plant integrated with TES

✓ Reduce boiler cycling, equipment damage, and potentially predicting future equipment failure

ALTO **Discrete (design) decisions**

✓ Optimal points of integration of TES

Rankine Cycle + TES

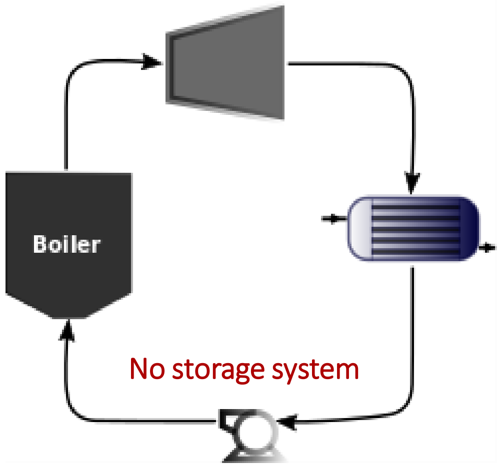
What storage material is the best and cheapest?

What is the best design for the storage system itself?

Where is the optimal integration point of the TES with the existing plant?

Optimization-based conceptual design of energy systems

- **Opportunity:**
  - Integrate existing energy systems with thermal energy storage (TES)
  - Charge and discharge storage operating cycles



Rankine Cycle
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Power plant integrated with TES

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Discrete (design) decisions

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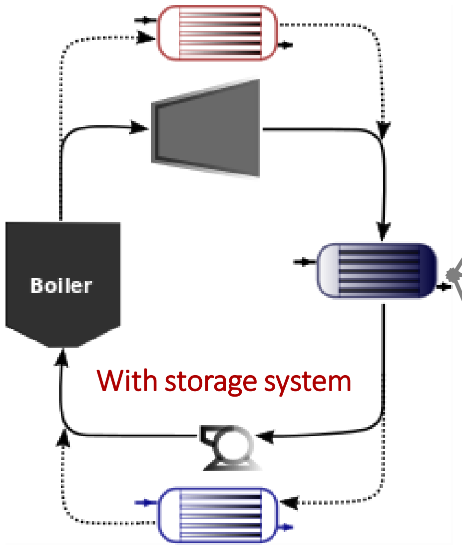

Rankine Cycle + TES

What storage material is the best and cheapest?

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Where is the optimal integration point of the TES with the existing plant?

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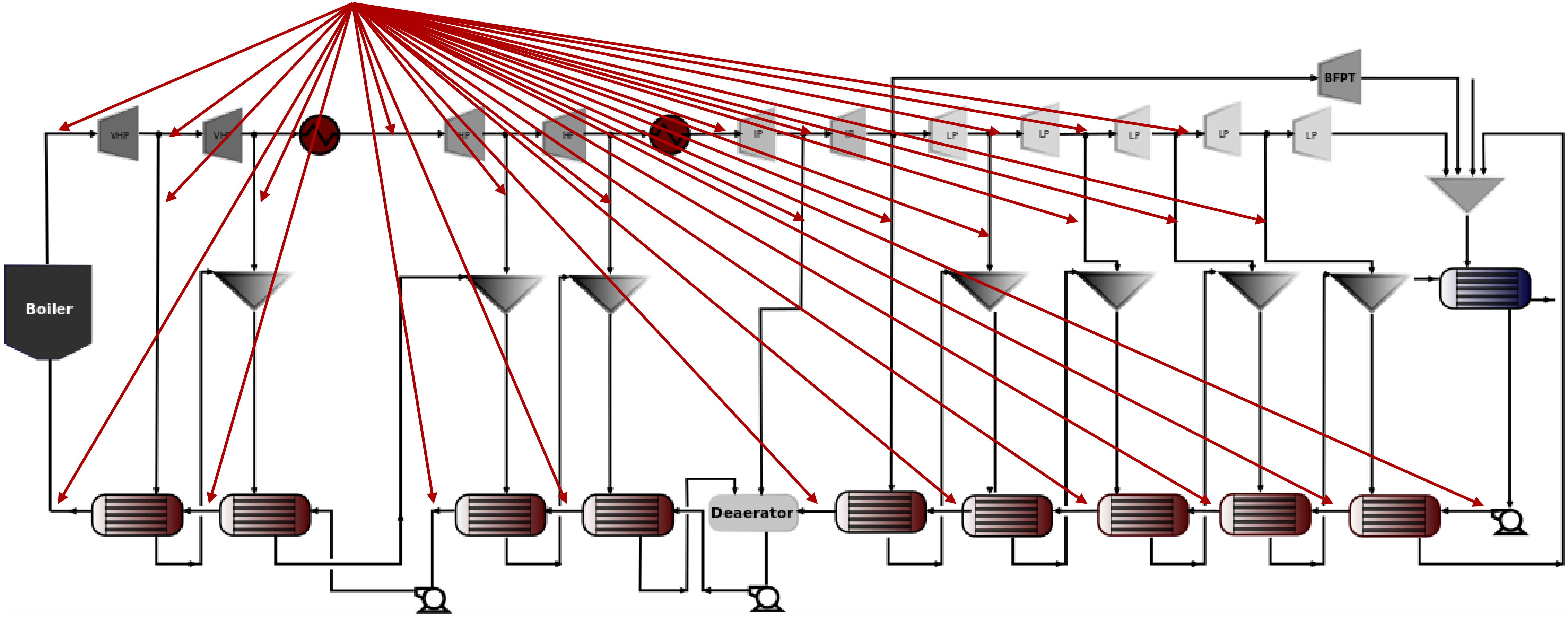
"Real" plants are significantly more complex

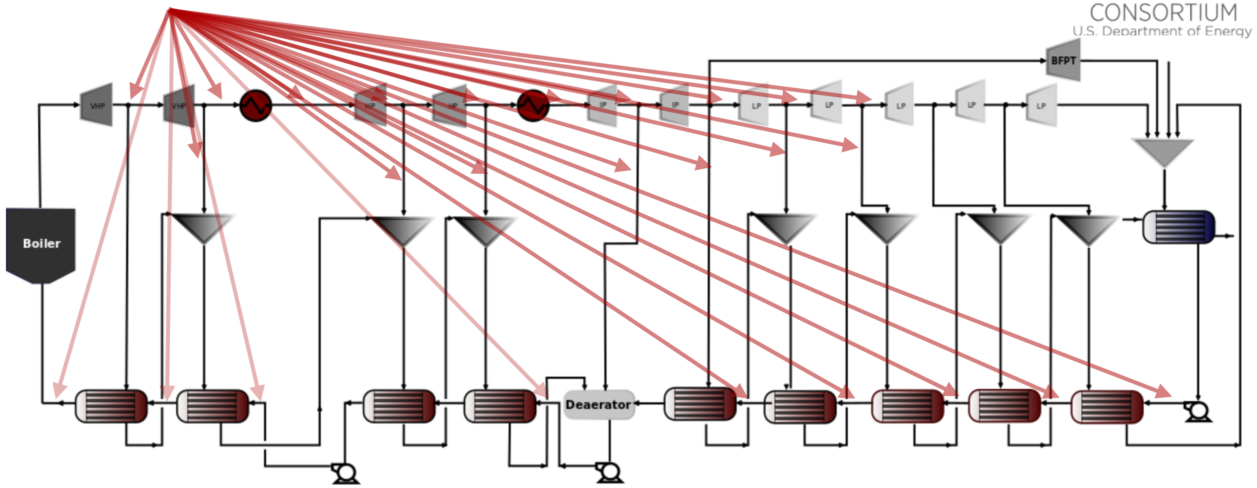
Where should we integrate the storage system?



Conceptual design through superstructure optimization

Strategies

1. Simulation: enumerate fixed designs
   - Unique model for each alternative
   - Explore limited integration choices
2. Optimization: encode design options into model
   - Explore all possible designs
   - MINLP[1] and GDP[2]



Review Optimization Problems

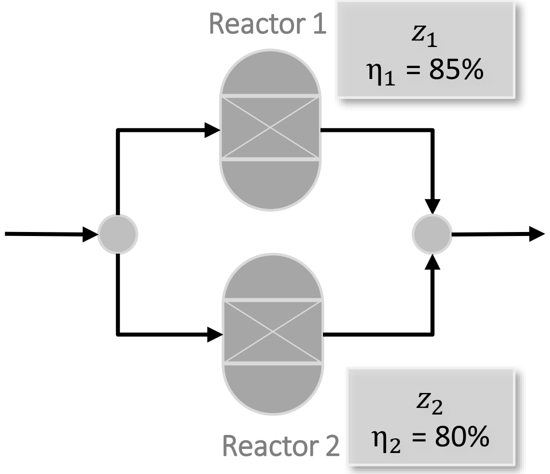
min O(x) ← objective

s.t. C(x) ← constraints

$x \in X$ ← variables

Variables: Integer → MINLP[1] (mixed integer solvers)

Constraints: Logic → GDP[2] (GDPopt solver)



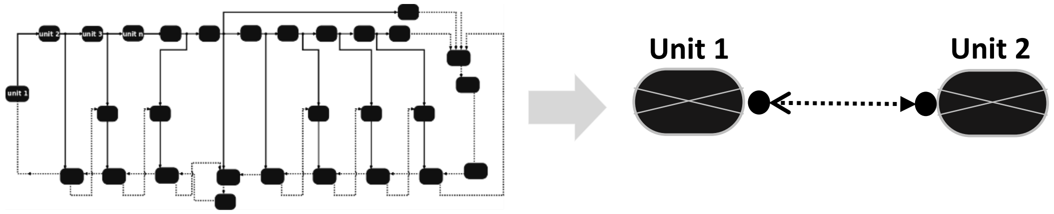
$$\begin{bmatrix} z_1 \\ \eta_1 = 85\% \\ h_1(x) = 0 \\ g_1(x) \leq 0 \end{bmatrix} \vee \begin{bmatrix} z_2 \\ \eta_2 = 80\% \\ h_2(x) = 0 \\ g_2(x) \leq 0 \end{bmatrix}$$

[1] Mixed Integer Linear and Nonlinear Programming, [2] Generalized Disjunctive Programming

Integrating TES design with thermal generator model

Conceptual Design in IDAES

- Use IDAES unit models and interconnections to create superstructures and rigorous models
- Use Generalized disjunctive programming (GDP) to incorporate discrete design decisions as disjunctions
- Use advanced cutting-edge solvers, such as **GDPopt**[1], to explore entire design space



Can be applied for designing storage systems for **fossil**, **nuclear**, and **geothermal energy systems**

Conceptual Design of Thermal Generator

Step 1: Construction of plant model

- Use IDAES unit model libraries and customized property packages
- Set initialization procedure by fixing inputs in models and propagating state variables

Step 2: Construction of GDP Model

- Two design superstructures, one for each operation cycle: Charge and discharge
- Include discrete design decisions as disjunctions using Pyomo *Disjunction* and *Disjunct* modeling objects

Step 3: Optimization Problem Formulation

- Mathematical model formulation to determine optimal points of integration of TES

x_i^*, z_j^*

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Modeling power plant

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Conceptual Design of Thermal Generator

Construction of base model

- Use of **IDAES Helm unit** model library
- Customized property packages: Solar and Hitec salt and Thermal oil
- Costing of unit operations into the flowsheet using IDAES unit costing methods
- **Initialization procedure**: Propagate state variables between the units

Construction of GDP Model

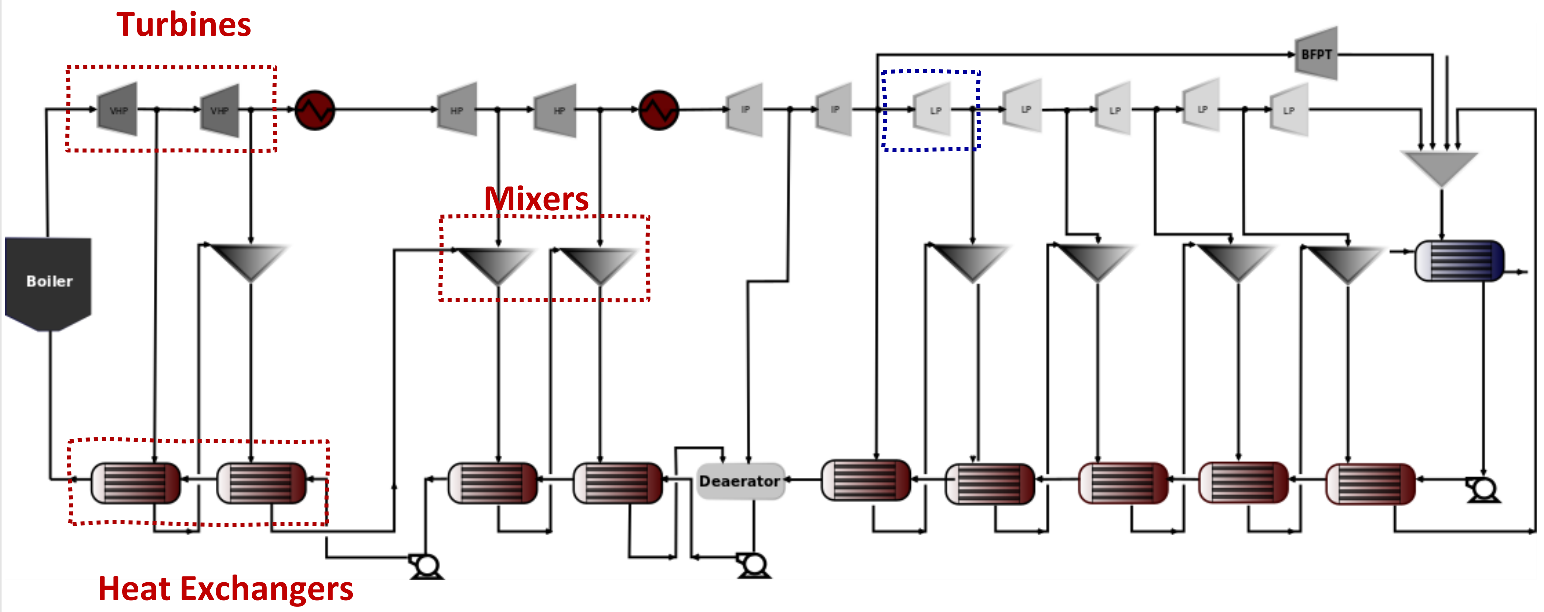
- Four discrete design decisions:
  1. Storage material
  2. Steam source
  3. Condensed steam return
  4. Cooler

Optimization Problem

$$\begin{aligned} \min \quad & C(x) && \leftarrow \text{charge cost} \\ \text{s.t.} \quad & h(x) = 0 && \leftarrow \text{model eqns.} \\ & \vee_{\forall d \in D} [z_{k,d}], \forall k \in K && \leftarrow \text{disjunctions} \\ & z_{k,d} = \{True, False\} && \leftarrow \text{Boolean var} \\ & x \in X, X \subseteq \mathbb{R}^n \end{aligned}$$

Solution

- GDPopt[1] solver using Gurobi and IPOPT



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Modeling power plant: Build the unit operations

GRID

Conceptual Design of Thermal Generator

Construction of base model

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Construction of GDP Model

- Four discrete design decisions:
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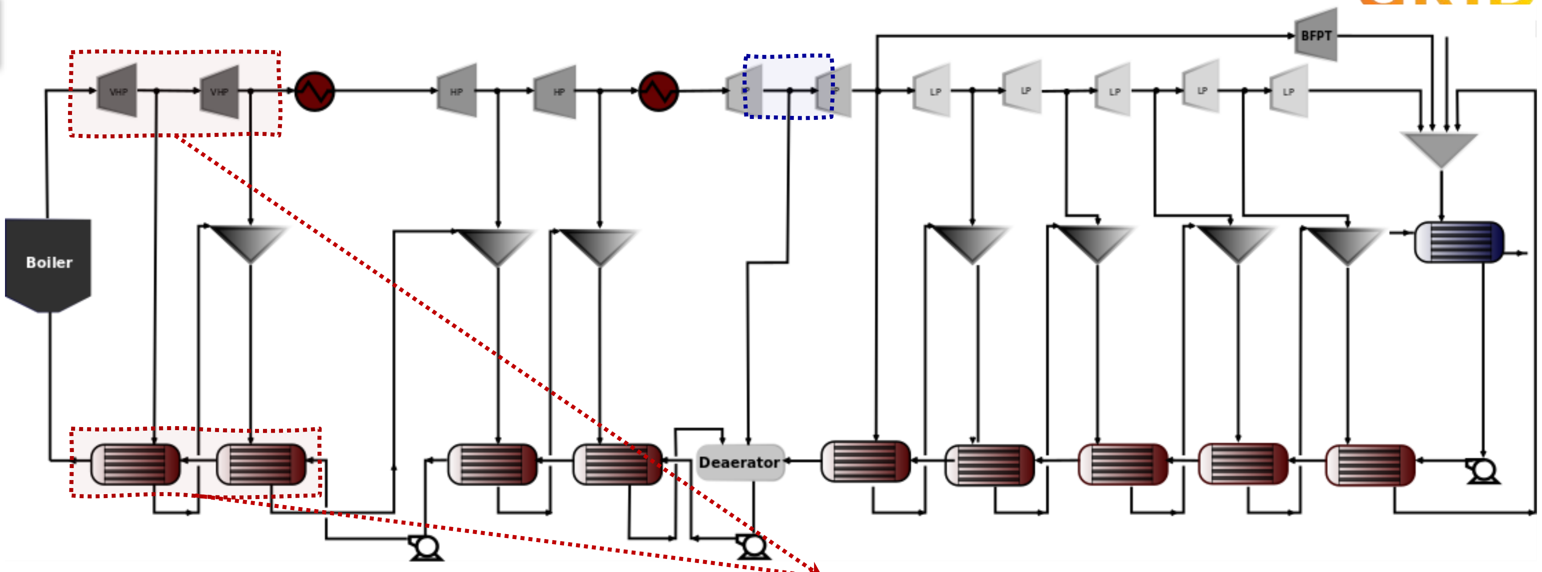
Optimization Problem

$$
\begin{aligned}
\min \quad & C(x) && \leftarrow \text{charge cost} \\
\text{s.t.} \quad & h(x) = 0 && \leftarrow \text{model eqns.} \\
& \vee_{\forall d \in D} [z_{k,d}], \forall k \in K && \leftarrow \text{disjunctions} \\
& z_{k,d} = \{True, False\} && \leftarrow \text{Boolean var} \\
& x \in X, X \subseteq \mathbb{R}^n &&
\end{aligned}
$$

Solution

- GDPopt[1] solver using Gurobi and IPOPT




```
m.fs.turbines = PressureChanger(m.TURBINES, default={
    "property_package": m.fs.prop_water,
    "compressor": False,
    "material_balance_type": MaterialBalanceType.componentTotal,
    "thermodynamic_assumption": ThermodynamicAssumption.isentropic,
})
m.fs.feed_water_heater = HeatExchanger(default={
    “delta_temperature_callback": delta_temperature_underwood_callback,
    “shell”: {”property_package”: m.fs.prop_water,
              “material_balance_type": MaterialBalanceType.componentTotal,
              “has_pressure_change": True},
    “tube": {”property_package”: m.fs.prop_water,
              “material_balance_type": MaterialBalanceType.componentTotal,
              “has_pressure_change": True}})
```

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

Modeling TES: Building charge superstructure

Conceptual Design of Thermal Generator

Construction of base model

- Use of **IDAES Helm unit** model library
- Customized property packages: Solar and Hitec salt and Thermal oil
- Costing of unit operations into the flowsheet using IDAES unit costing methods
- **Initialization procedure**: Propagate state variables between the units

Construction of GDP Model

- Four discrete design decisions:
  1. Storage material
  2. Steam source
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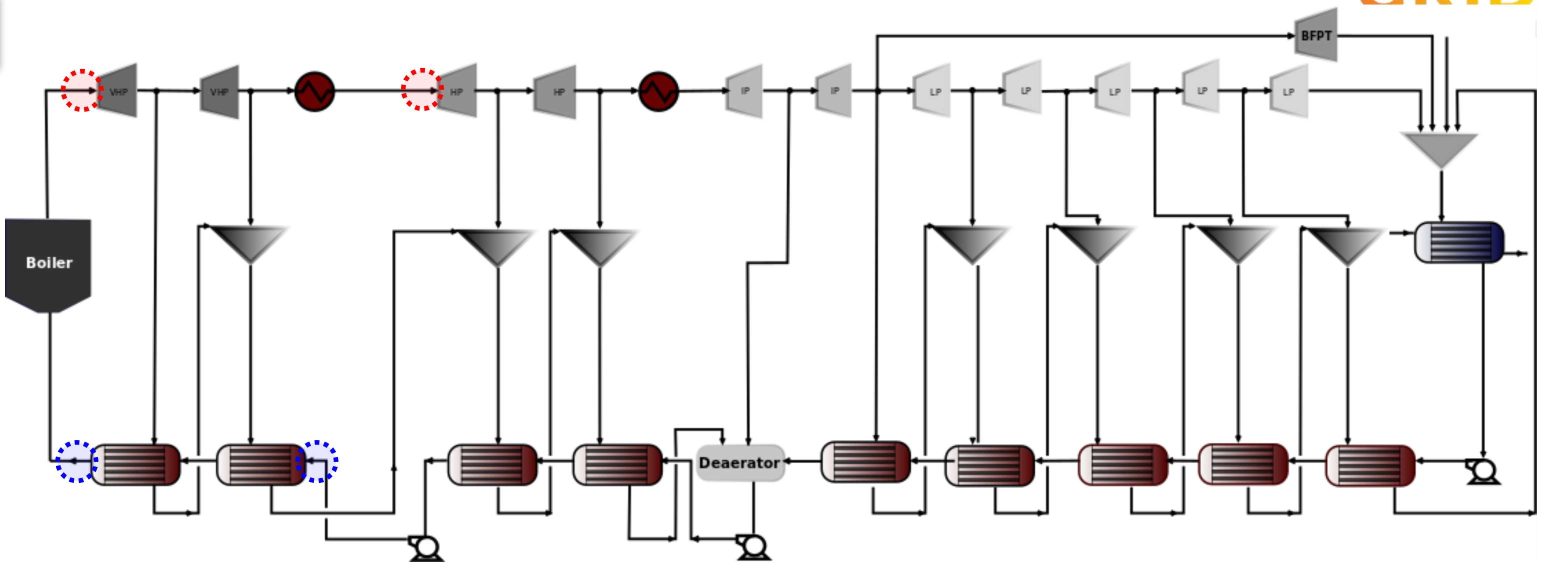
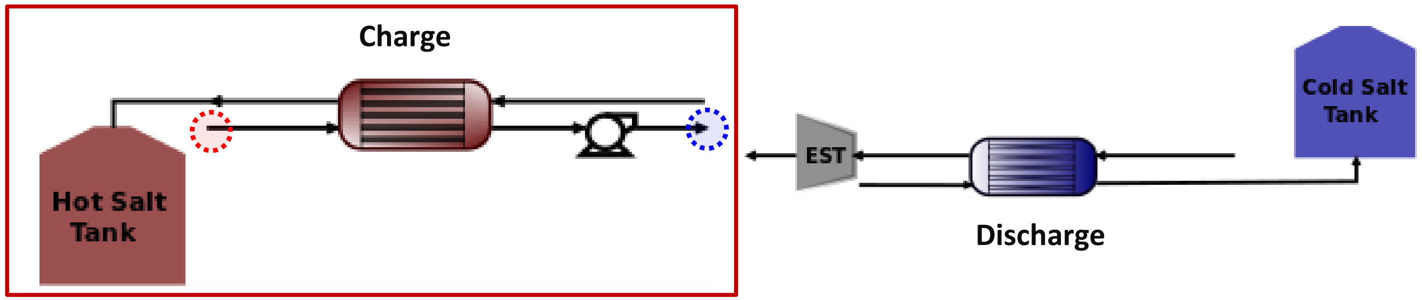
Optimization Problem

$$
\begin{aligned}
\min \quad & C(x) && \leftarrow \text{charge cost} \\
\text{s.t.} \quad & h(x) = 0 && \leftarrow \text{model eqns.} \\
& \bigvee_{\forall d \in D} [z_{k,d}], \forall k \in K && \leftarrow \text{disjunctions} \\
& z_{k,d} = \{True, False\} && \leftarrow \text{Boolean var} \\
& x \in X, X \subseteq \mathbb{R}^n &&
\end{aligned}
$$

Solution

- GDPopt[1] solver using Gurobi and IPOPT





Thermal energy storage system (TES): Units in charge cycle (right) and discharge cycle (left)

Modeling TES charge cycle: Define disjunctions

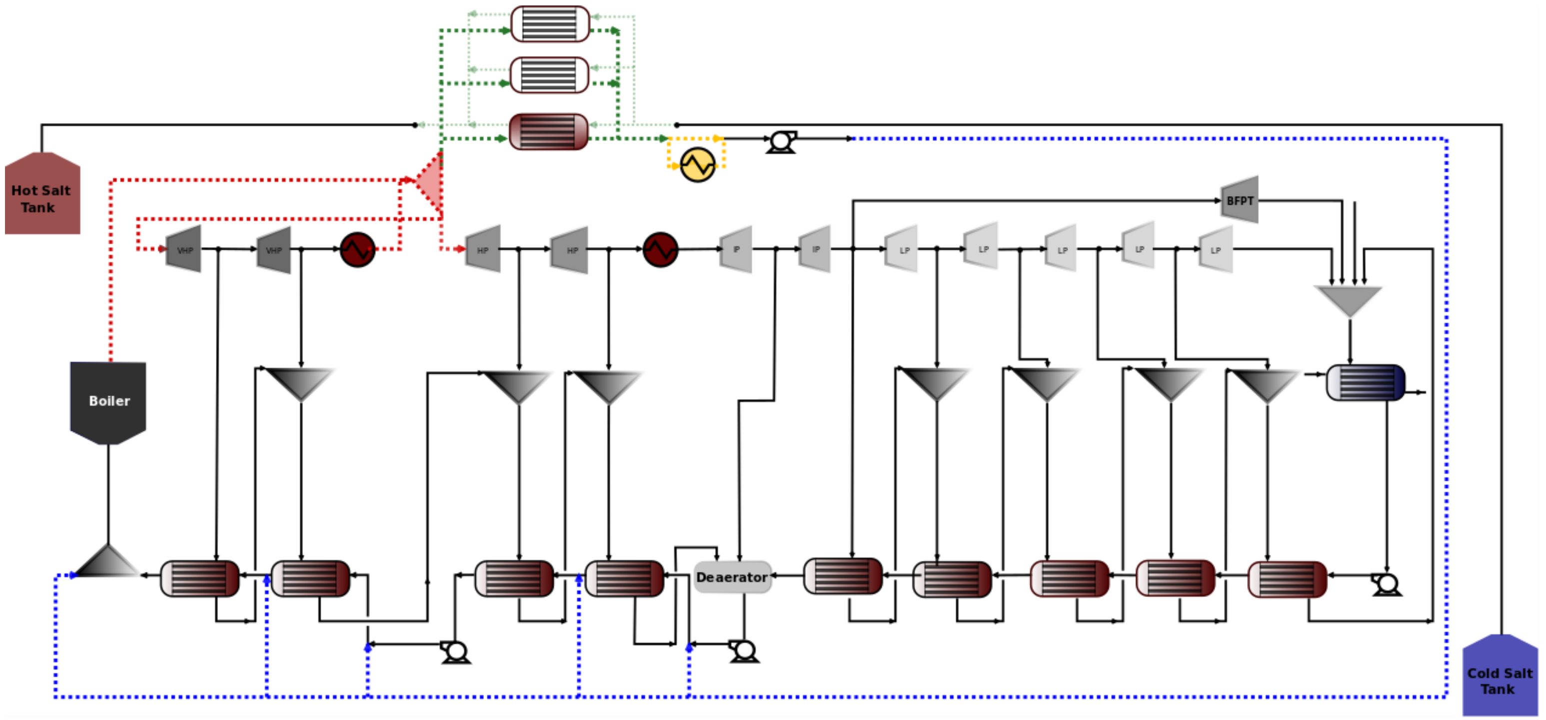
Conceptual Design of Thermal Generator

Construction of base model
- Use of **IDAES Helm unit** model library
- Customized property packages: Solar and Hitec salt and Thermal oil
- Costing of unit operations into the flowsheet using IDAES unit costing methods
- **Initialization procedure**: Propagate state variables between the units

Construction of GDP Model
- Four discrete design decisions:
  1. Storage material: Solar or Hitec salt and thermal oil storage heat exchangers
  2. Steam source: Very high and high pressure steam from two sources
  3. Condensed steam return: five alternative points to return condensed steam to the cycle
  4. Cooler: Use or not use a cooler after the storage heat exchanger

Optimization Problem
- Mathematical formulation of GDP model

Solution
- GDPopt[1] solver using Gurobi and IPOPT



Modeling TES charge cycle: Implement disjunctions

Conceptual Design of Thermal Generator

Construction of base model

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Construction of GDP Model

- Four discrete design decisions:
  1. Storage material

$$\begin{bmatrix} z_{1,1} \\ HXC_{Solar\ Salt} \end{bmatrix} \vee \begin{bmatrix} z_{2,1} \\ HXC_{Hitec\ Salt} \end{bmatrix} \vee \begin{bmatrix} z_{3,1} \\ HXC_{Thermal\ Oil} \end{bmatrix}$$

  2. Steam source

$$\begin{bmatrix} z_{1,2} \\ F_{in}^{VHP\ Split} = F_{out}^{Boiler} \\ F_{in1}^{HXC_i} = F_{out2}^{VHP\ Split} \end{bmatrix} \vee \begin{bmatrix} z_{2,2} \\ F_{in}^{HP\ Split} = F_{out}^{Reheater\ 1} \\ F_{in1}^{HXC_i} = F_{out2}^{HP\ Split} \end{bmatrix}$$

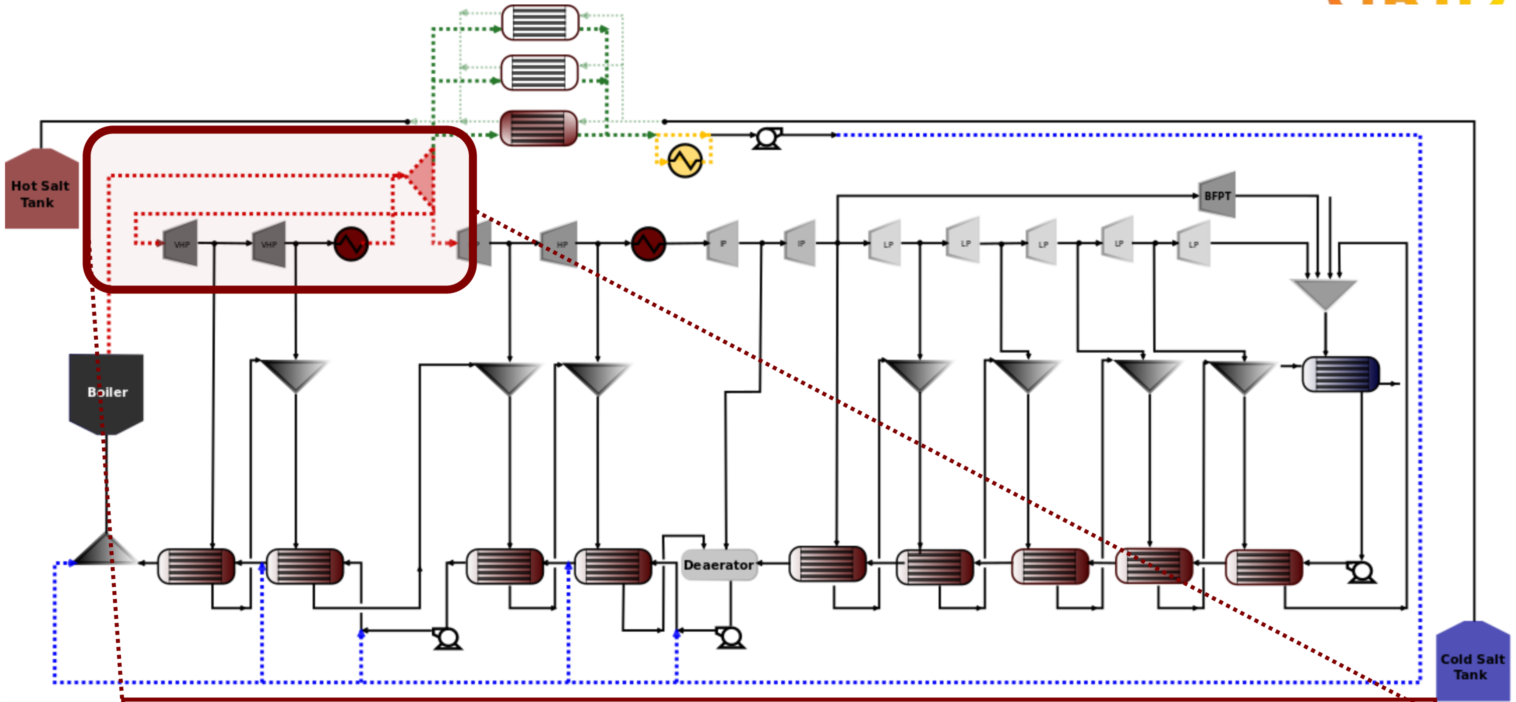
  3. Condensed steam return …

Optimization Problem

- Mathematical formulation of GDP model

Solution

- GDPopt[1] solver using Gurobi and IPOPT




```
m.fs.steam_source_disjunction = Disjunction(expr=[
    [ m.fs.hxc.inlet_1.flow_mol[0] == m.fs.vhp_split.to_hxc.flow_mol[0],
      m.fs.hxc.inlet_1.pressure[0] == m.fs.vhp_split.to_hxc.pressure[0],
      m.fs.hxc.inlet_1.enth_mol[0] == m.fs.vhp_split.to_hxc.enth_mol[0]
    …],
    [ m.fs.hxc.inlet_1.flow_mol[0] == m.fs.hp_split.to_hxc.flow_mol[0],
      m.fs.hxc.inlet_1.pressure[0] == m.fs.hp_split.to_hxc.pressure[0],
      m.fs.hxc.inlet_1.enth_mol[0] == m.fs.hp_split.to_hxc.enth_mol[0]],
    …])
```

TES charge cycle superstructure model

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Conceptual Design of Thermal Generator

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Construction of GDP Model

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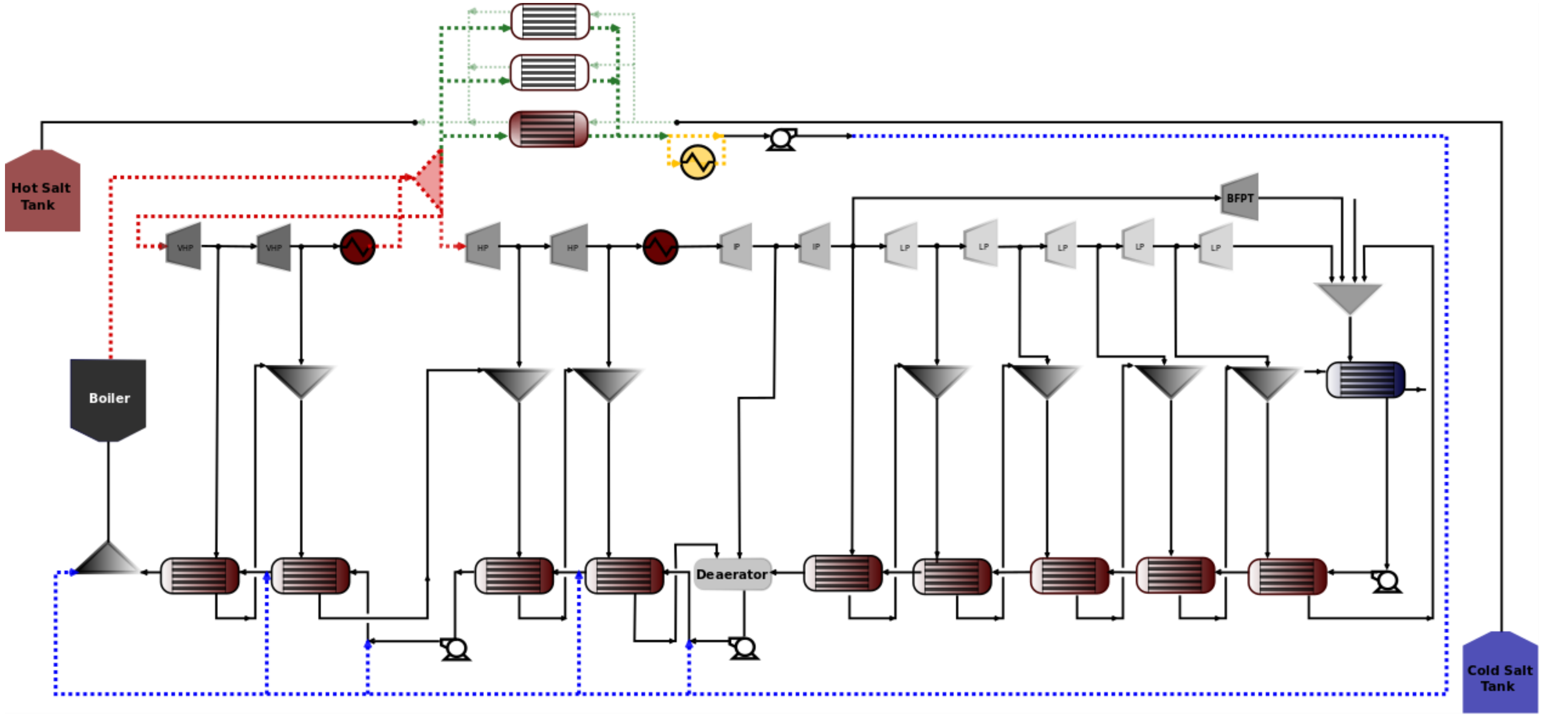
Solution

- GDPopt[1] solver using Gurobi and IPOPT



60 total process configurations to consider!

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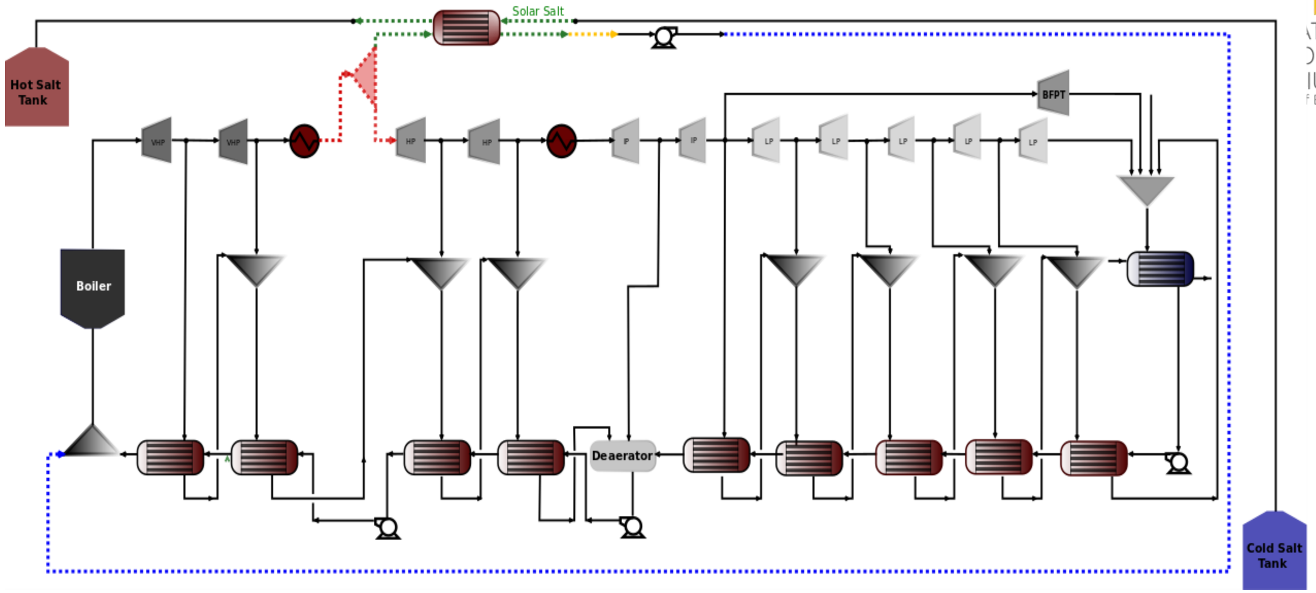
[1] Chen, Q., Johnson, E. S., Bernal, D. E., Valentin, R., Kale, S., Bates, J., ... & Grossmann, I. E. (2021). Pyomo. GDP: an ecosystem for logic based modeling and optimization development. Optimization and Engineering, 1-36.

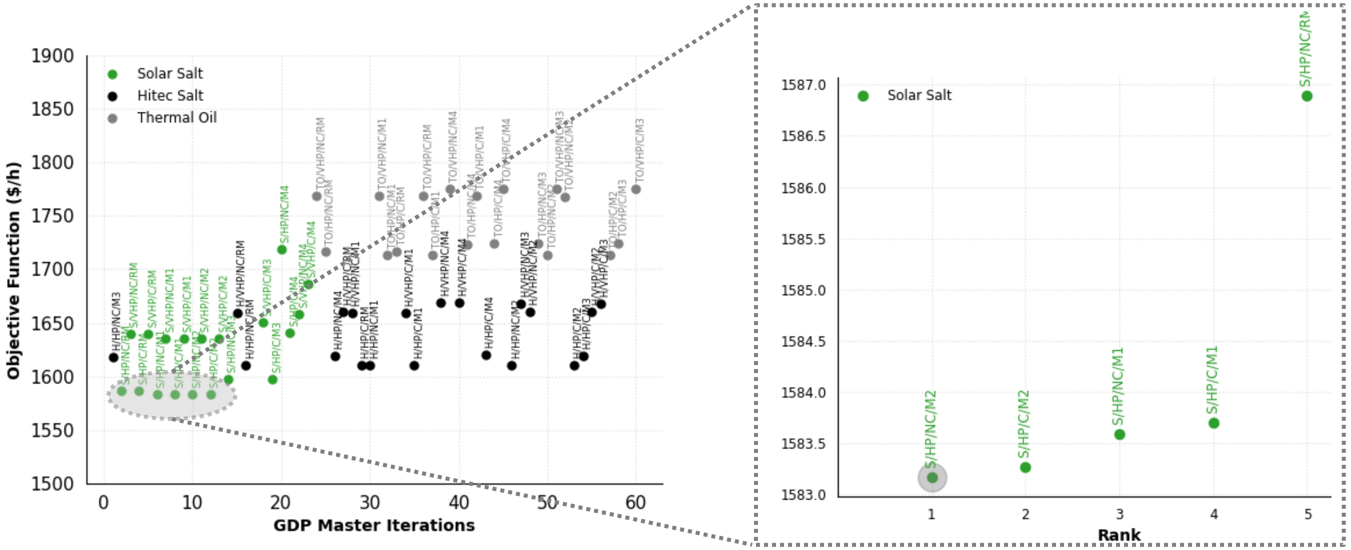
Charge cycle optimal design

Design Decisions

- Optimal design decisions:
  - ✓ Storage material: Solar salt
  - ✓ Steam source: Reheater 1
  - ✓ Condensed steam return: Boiler inlet
  - ✓ No cooler
- Power plant is producing 400 MW of power at high efficiency



- **Key trends:**
  - Five designs identified Solar salt as the storage medium
  - Selection of HP over VHP steam source
- **Solver performance:**
  - 60 alternatives explored in ~882 seconds
  - Model statistics: 795 constraints and 729 variables



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TES discharge cycle superstructure model

Conceptual design of Thermal Generator

Construction of base model

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- Customized property packages: Solar and Hitec salt and Thermal oil
- Costing of unit operations into the flowsheet using IDAES unit costing methods
- **Initialization procedure**: Propagate state variables between the units

Construction of GDP Model

- One discrete design decision:
  1. Condensed steam source: Feed water heater train

Optimization Problem

$$
\begin{aligned}
\min\ & C(x) && \leftarrow \text{charge cost} \\
\text{s.t.}\ & h(x) = 0 && \leftarrow \text{model eqns.} \\
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\end{aligned}
$$

Solution

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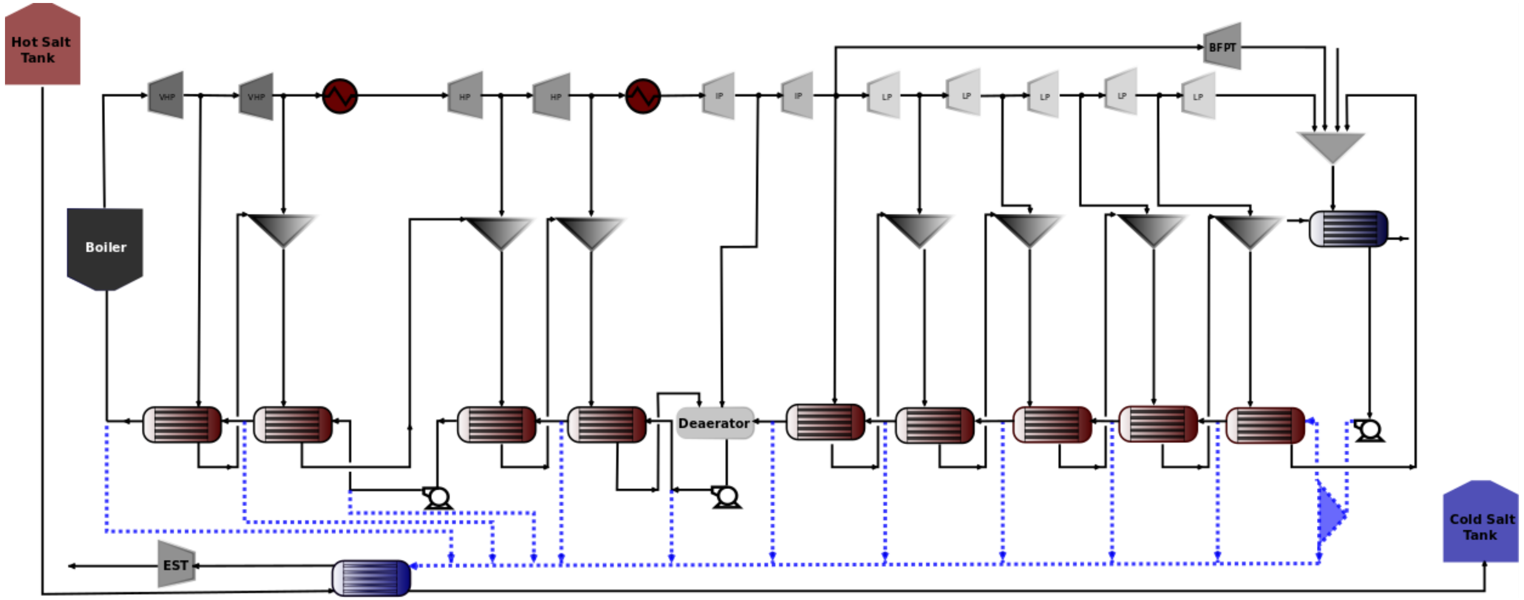

11 total process configurations to consider!

DISPATCHES
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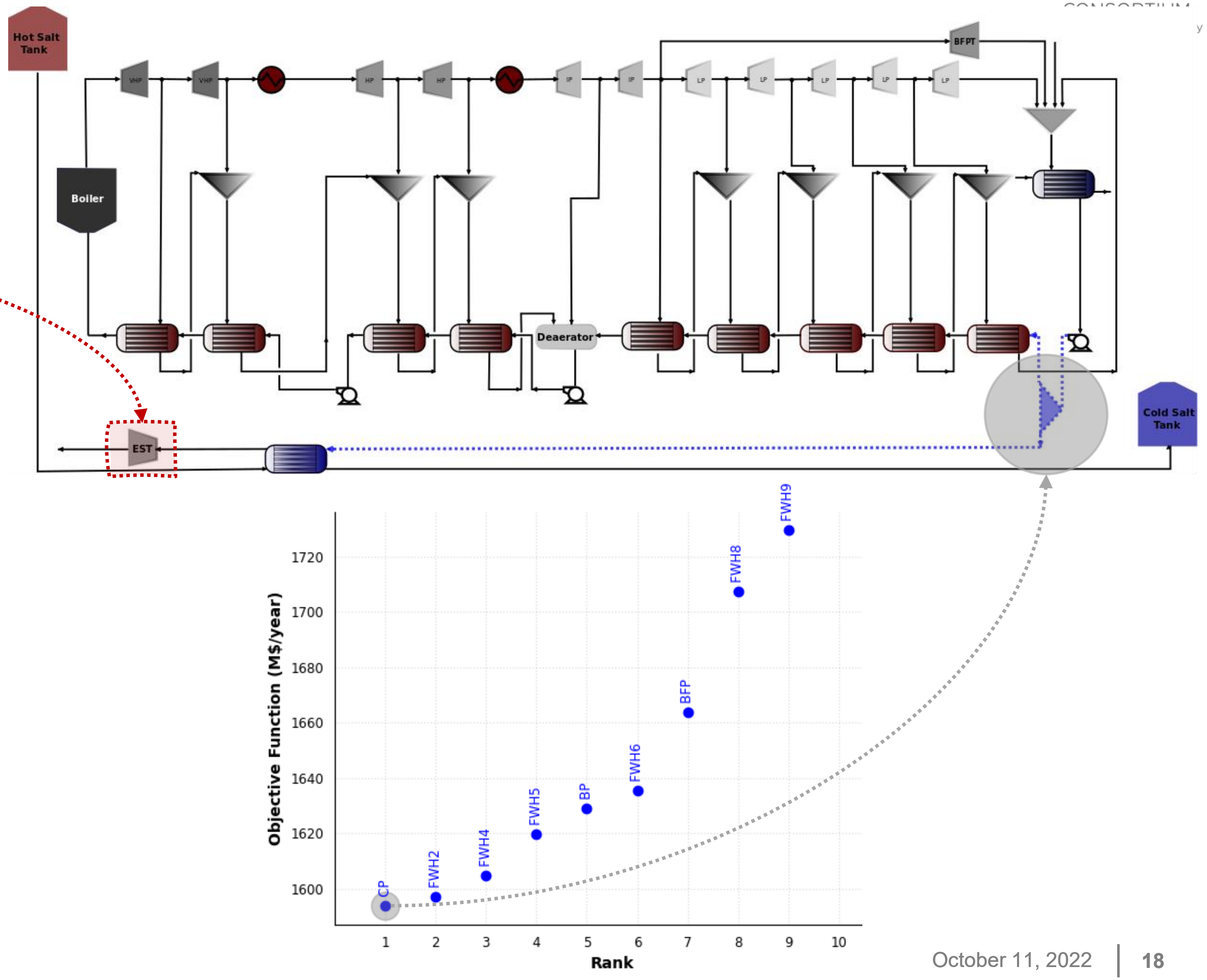
[1] Chen, Q., Johnson, E. S., Bernal, D. E., Valentin, R., Kale, S., Bates, J., ... & Grossmann, I. E. (2021). Pyomo. GDP: an ecosystem for logic based modeling and optimization development. Optimization and Engineering, 1-36.

Discharge cycle optimal design

Discrete Design Decisions

- Optimal design:
  - ✓ Condensed steam source: From condenser pump
- Reheated steam used to produce **36 MW** of extra power using a turbine within the discharge cycle
- Integrated power plant with discharge heat exchanger produces maximum power of 436 MW



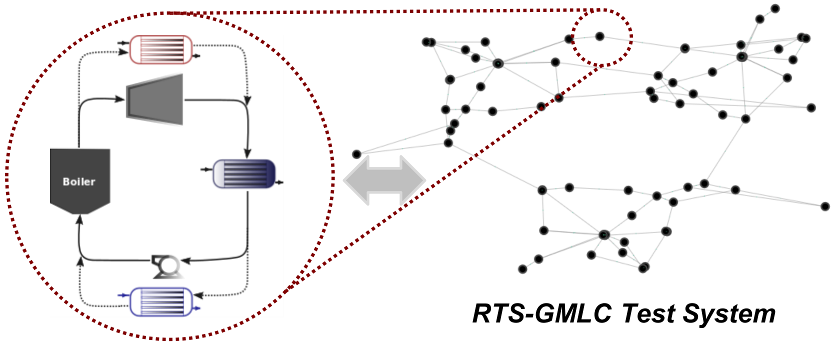
- **Key assumptions from charge cycle:**
  - Solar salt as the storage medium
  - Hot salt temperature (~550C)
- **Solver performance:**
  - 11 alternatives explored in ~352 seconds
  - Model statistics: 916 constraints and 568 variables

Summary

- IDAES unit models, disjunctive superstructures, and custom algorithms enable the ***simultaneous process configuration and optimization*** of process operating conditions
- Optimal design of thermal generator integrated with thermal energy storage:
  - Demonstrated a simple workflow by using an existing IDAES ultra-supercritical power plant model within the GDPopt framework to construct two design superstructures
    - No new model is required to switch to "design mode"

Future work

- Include discharge steam in Carbon Capture System as a potential design option
- Extend analysis beyond cycle net efficiency as the design objective, and instead, design for:
  - Market participation (pricetaker assumption)
  - Dynamic operation (multi-period assumption with revenue)
  - Grid adoption (double-loop approach)



RTS-GMLC Test System

GRID MODERNIZATION LABORATORY CONSORTIUM
U.S. Department of Energy

Any questions?

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