Tracking No: **INL/MIS-14-31053**

Process Integration & Optimization Using Dynamic Systems Models

Key words: **energy systems** integration & **HiL** simulation, dynamic energy systems **optimization**, predictive/safety critical supervisory & **resilient controls**, smart **energy grids**/microgrids

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Objectives

- Innovation
- Collaboration
- HiL demonstration

AIChE CAST Webinar Series
January 14, 2014

Idaho National Laboratory

Outline

- **Motivation**
- Hybrid Energy Systems (HES)
- Modeling Issues
- Co-simulation Issues
- Optimization Issues
- Dynamic Analyses with Casual Models
- Dynamic Analyses with Acasual Models
- Optimization Studies with Acasual Models
- Conclusion

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The world is powered by many energy sources…

Traditional Energy

- Coal
- Gas turbines
- Steam turbines
- Gas engines
- Diesel engines
- Nuclear

Renewable Energy

- Wind
- Solar Thermal
- Solar PV
- Geothermal
- Biomass
- Waste heat recovery
- Hydro

Energy Storage

- Batteries
- Compressed air
- Pumped hydro
- Chemical fuels – H_2, CH_4

Output Commodities

- Electricity
- Chemical products
- Synthetic fuels
- Heat
- Clean water

[] …are there COMBINATIONS or HYBRIDIZATIONS that are particularly attractive?

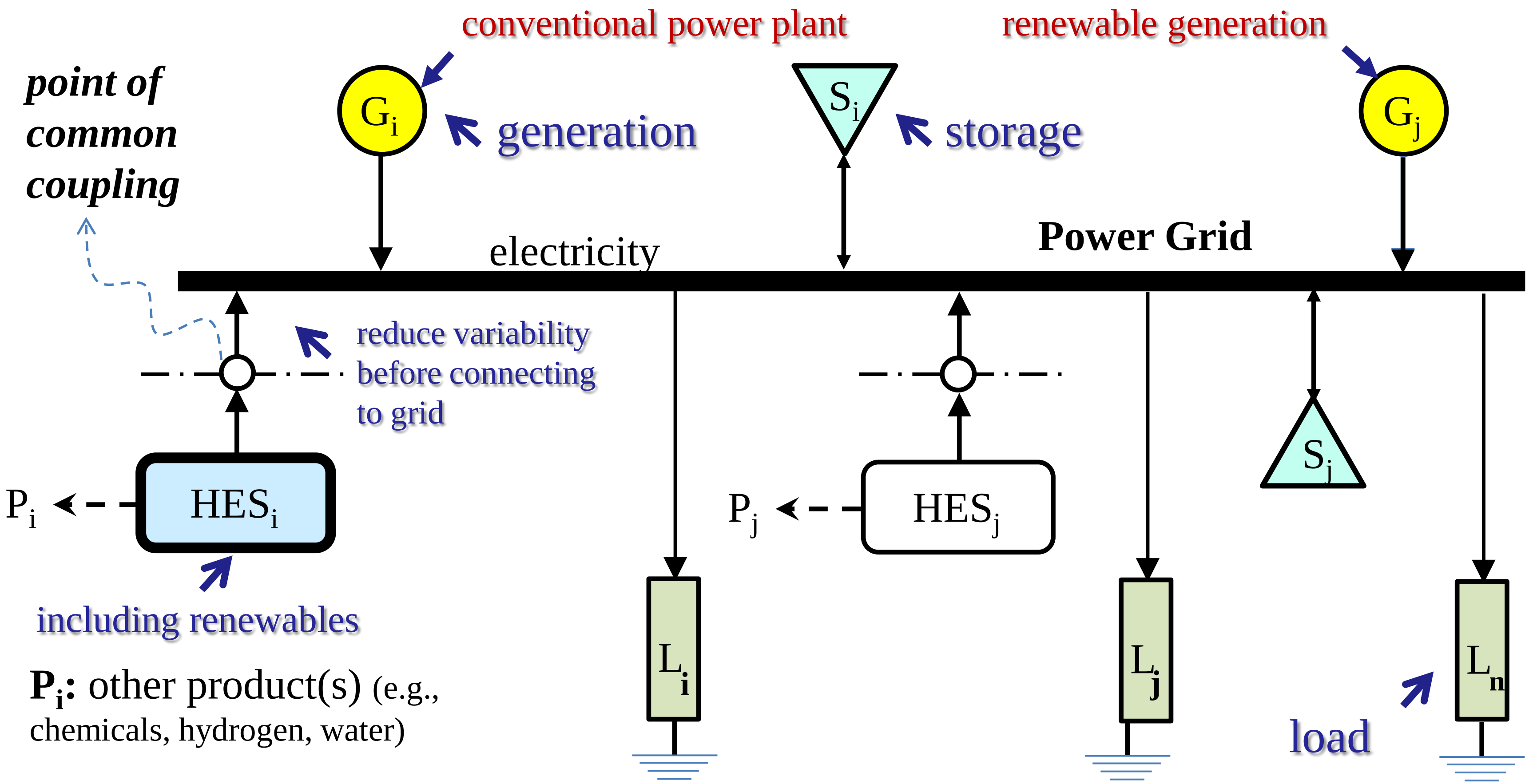
[] …how are reliability and environmental stewardship affected by selected configurationS?

[] …can nuclear energy complement or compensate for renewable energy build-out and emerging grid dynamics?

[] …what is the role of next generation nuclear reactors?

[] …how does system integration change energy storage needs?

***Distributed Solution**: Hybrid Energy Systems (HES)*



- Facilitate **effective and efficient integration of clean & sustainable energy solutions**;
- Enhance both **power & energy management**, in addition to reliability and **security**;
- Extended **electrical** & **thermal options for variability management**, thus reducing stress on power grid;
- Promote **usage of carbon sources** and **reduce environmental impact**;
- Leading to regional/nation-wide "**energy grids**";
- Support smooth integration of diverse energy sources and products within **existing infrastructures**;

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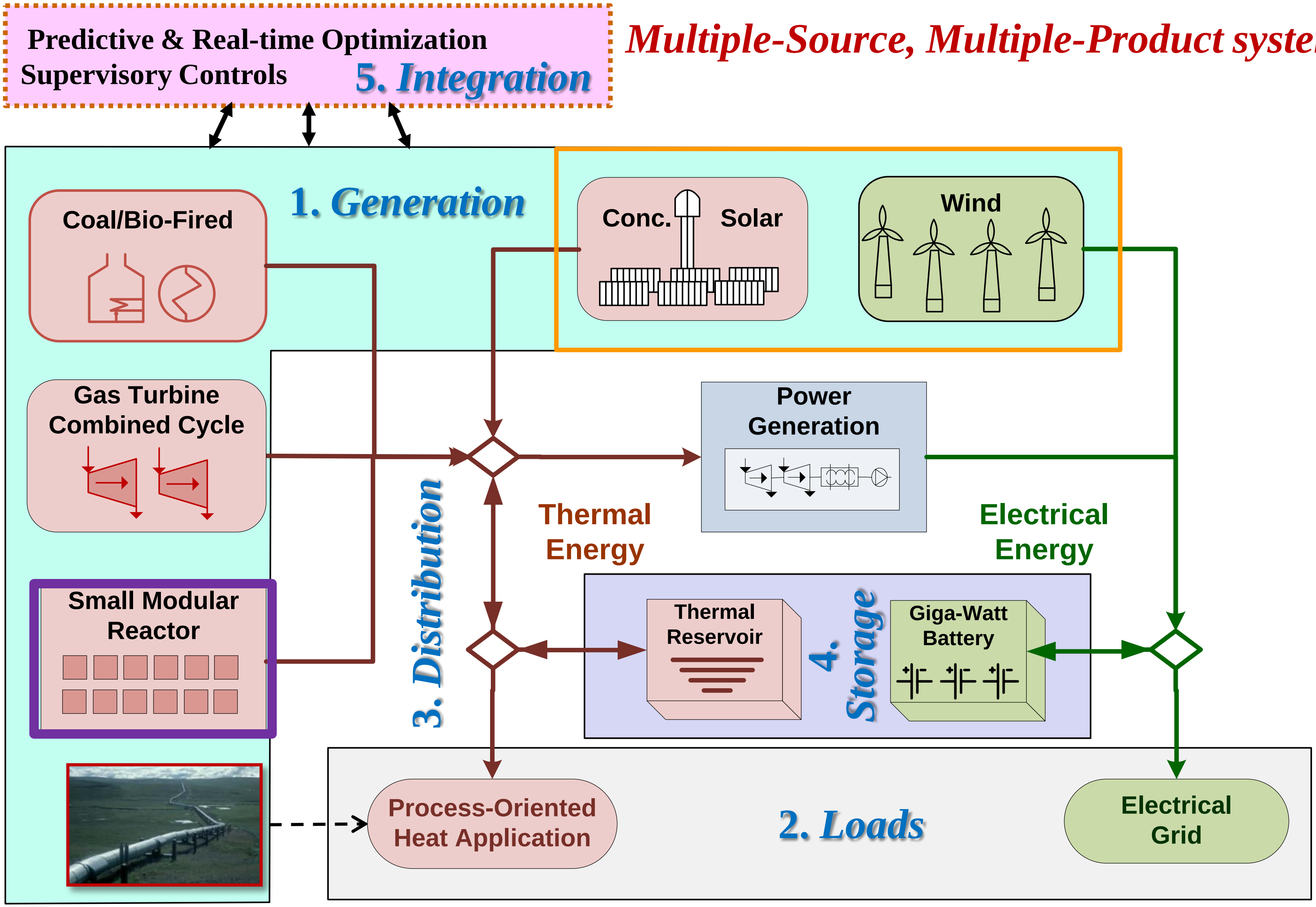
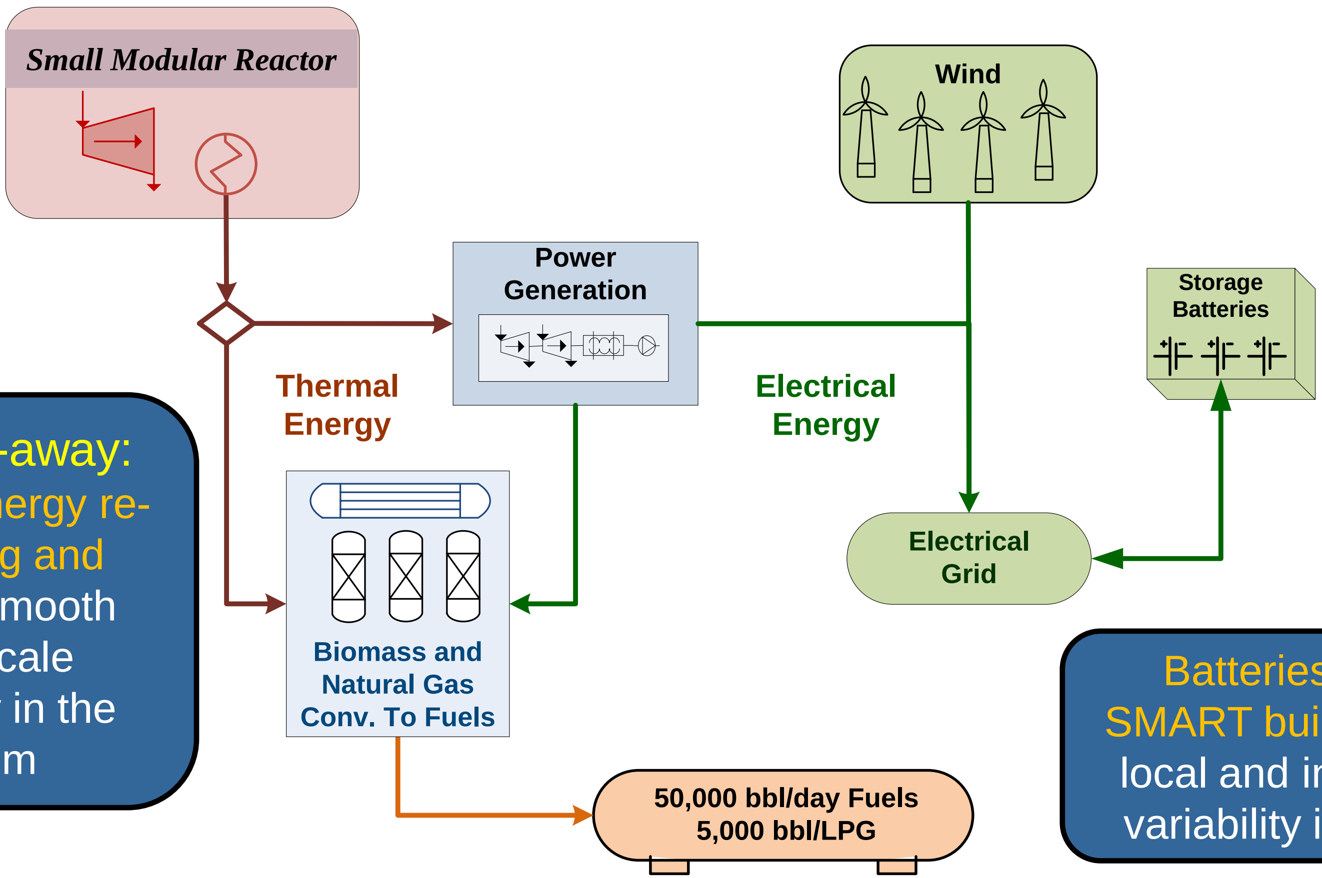
Hybrid Energy System (HES): A Multiple-Input, Multiple-Output (MIMO) system



HYBRID (engine & battery) CARS → HYBRID (nuc, ren, chem, grid) ENERGY SYSTEMS

Keys to energy systems integration…

- **Dynamic Integration**
- Grid Stabilization
- **Energy Storage**
- **Capital Efficiency**
- Resource/system optimization
- **Monitoring & Controls**



Key take-away: Thermal energy re-purposing and storage smooth large-scale variability in the system

Batteries, EV's and SMART buildings smooth local and instantaneous variability in the system

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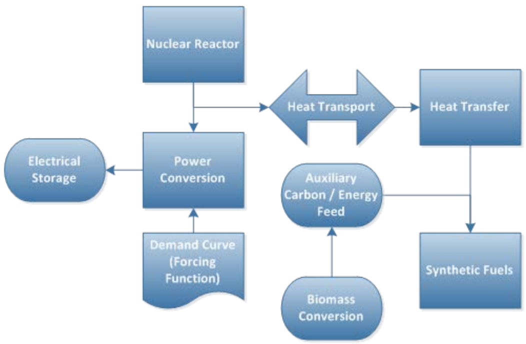
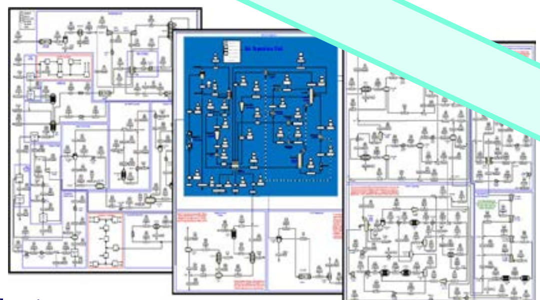
Graded Approach to Identify, Design, Analyze, Test & Optimize Advanced Energy Solutions

Energy Solution Identification based on Local/Global Requirements & Constraints



- Batch analysis
- High-level requirements and resources analysis

Feasibility, Life-Cycle & Economic Assessment of Identified Energy Solutions



- Steady-state analysis
- Time-average analysis

"A system-centric approach to devise efficient, sustainable & resilient energy solutions"

Dynamic Analysis, Testing & Optimization of Selected Energy Solutions

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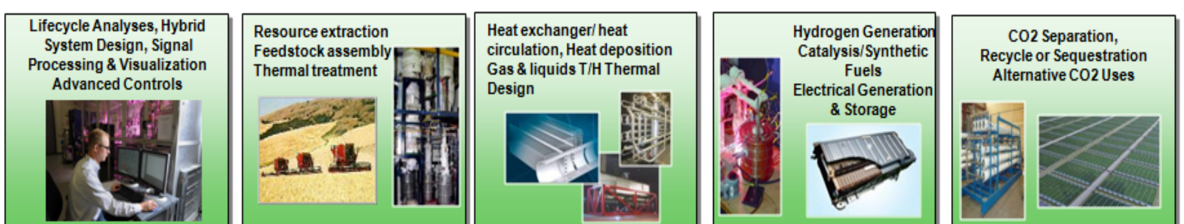
- Dynamic Performance/Cost Analysis
- Dynamic Integrated Equipment Analysis
- Multidimentional Co-optimization
- **HiL testing & demonstration**

Energy Systems Sustainable Integration



Systems Integration, Analyses, Optimization, Monitoring, Control

Feedstock Extraction & Processing

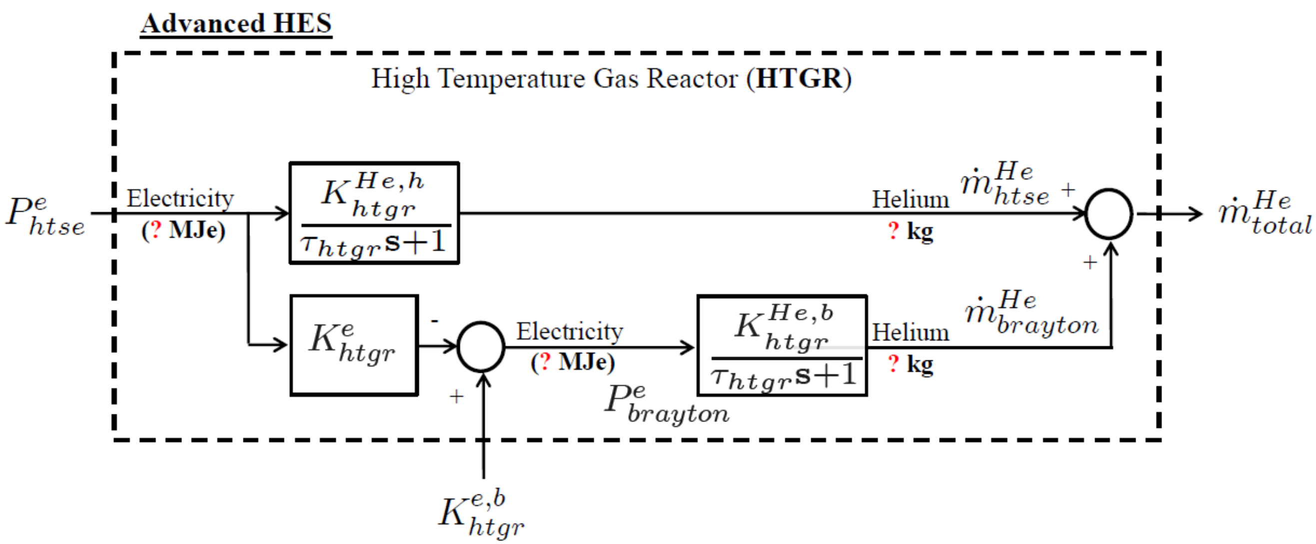
Energy Transfer

Energy Storage

Byproduct Management

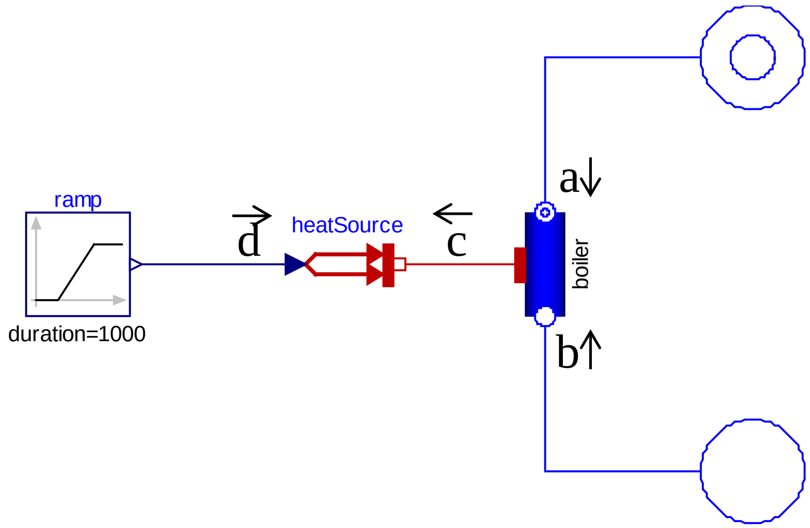
Causal Modeling: Nuclear Reactor

- Electrical and thermal energy flows are modeled as signals modified by transfer functions.
- In causal modeling, energy flows are unidirectional (inputs and outputs must be specified).
- Transfer functions are derived from conducting mass and energy balance, and gains are calculated using efficiency and unit conversion values.



Acausal Modeling: Nuclear Reactor

- In contrast to causal (e.g., signal-based), acausal physics-based models solves governing equations for the actual physical phenomena in the system.
- In acausal models, equations are solved without regard for whether variables are inputs or outputs. Thus, equality relationships are interpreted as mathematical equalities as opposed to assignments.



Heat source:

$$-\dot{Q}_c = \dot{Q}_d\left(1 + \alpha\left(T - T_{ref}\right)\right)$$

Laminar flow:

$$\Delta P = -\rho g \Delta z + \Delta P_{nominal}\frac{\dot{m}}{\dot{m}_{nominal}}$$

Mass balance:

$$\dot{m}_a + \dot{m}_b = 0$$

Energy balance:

$$h_a \dot{m}_a + h_b \dot{m}_b = \dot{Q}_c$$

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Requirements for Physical Systems Modeling, Co-simulation, Optimization

1. **Acausal/declarative: capable of solving problems of any structure**
   - No a priori need to identify givens (inputs) and unknowns (outputs)
   - Formulation independent of actual boundary conditions
   - Context-independent form, without caring about actual solution algorithm
   - Facilitate model reusability
2. **Multi-domain: effective integration of simulated models and physical systems from diverse disciplines**
   - Complete integrated simulation including thermo-hydraulics, electrical, mechanical, and chemical dynamics of diverse energy conversion systems
   - Support HiL demonstrations
3. **Open: allow construction and/or modification of existing component modules to accommodate specific needs**
4. **Dynamic & Hybrid**: emphasis on dynamic analysis to evaluate and accommodate issues related to flexible operation and variable generation
   - Dynamic performance and cost analysis, monitoring and controls, sensitivity, robustness, what-if analysis, optimization
   - Time-driven plus event-driven modeling

"Selected Solution: Modelica"

5. **Non-proprietary: Ease of collaboration through open licensing**

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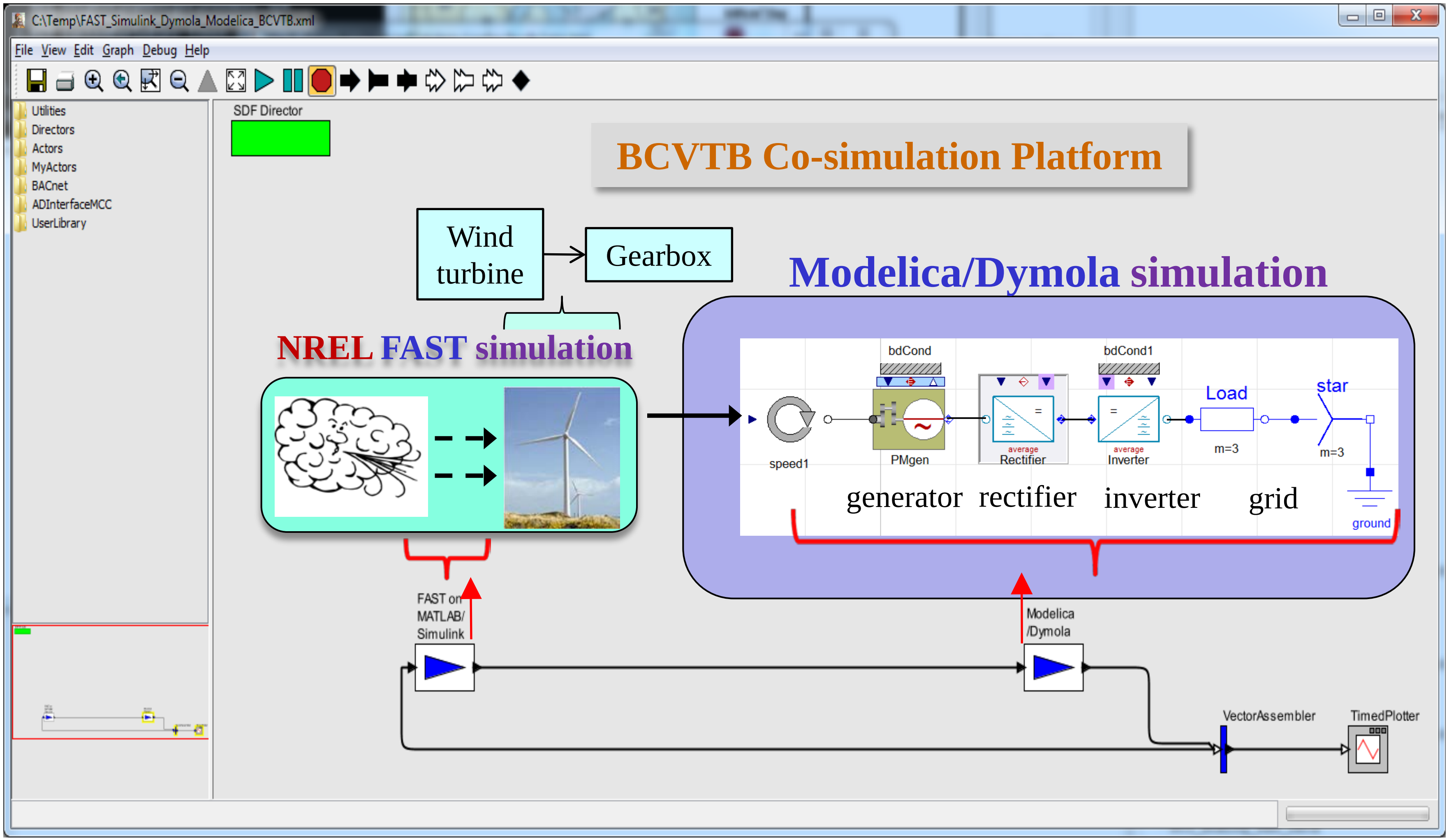
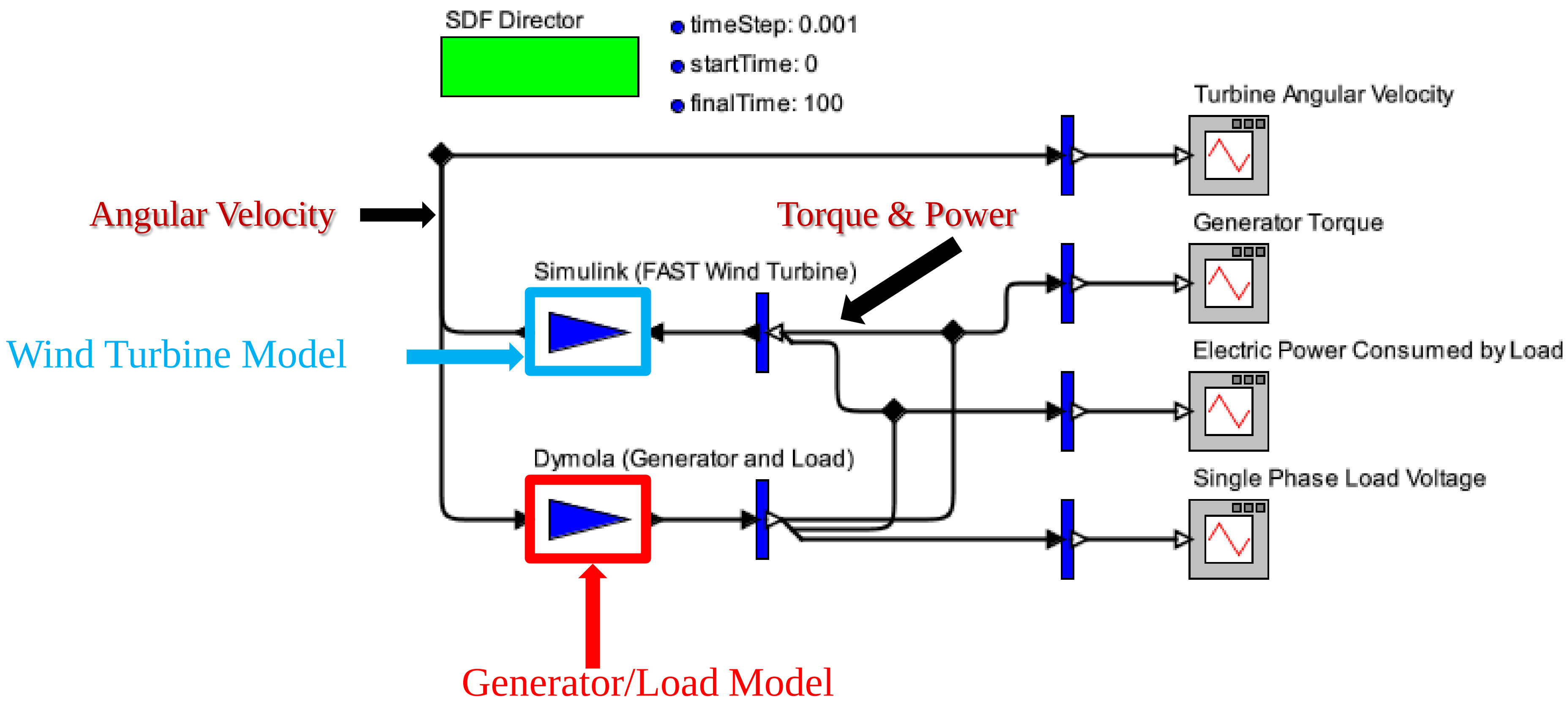
Co-Simulation of Wind Turbine & Generator Models (1)

Shows from wind velocity to wind turbine, gearbox, generator, rectifier, inverter, grid/load



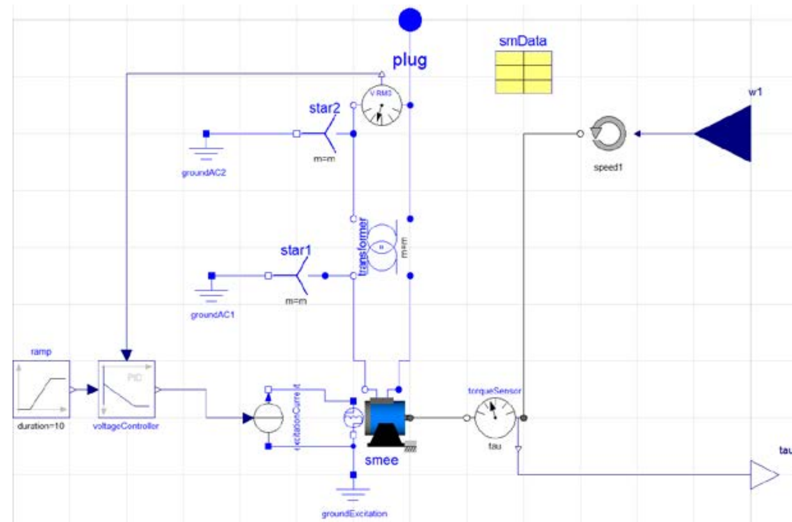
Co-Simulation of Wind Turbine & Generator Models (2)

Building Controls Virtual Test Bed (BCVTB)

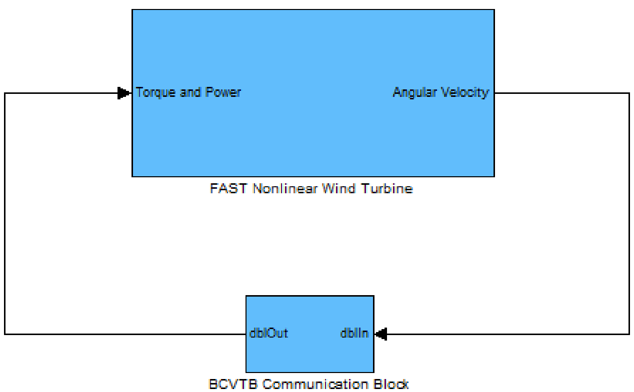


Co-Simulation of Wind Turbine & Generator Models (3)

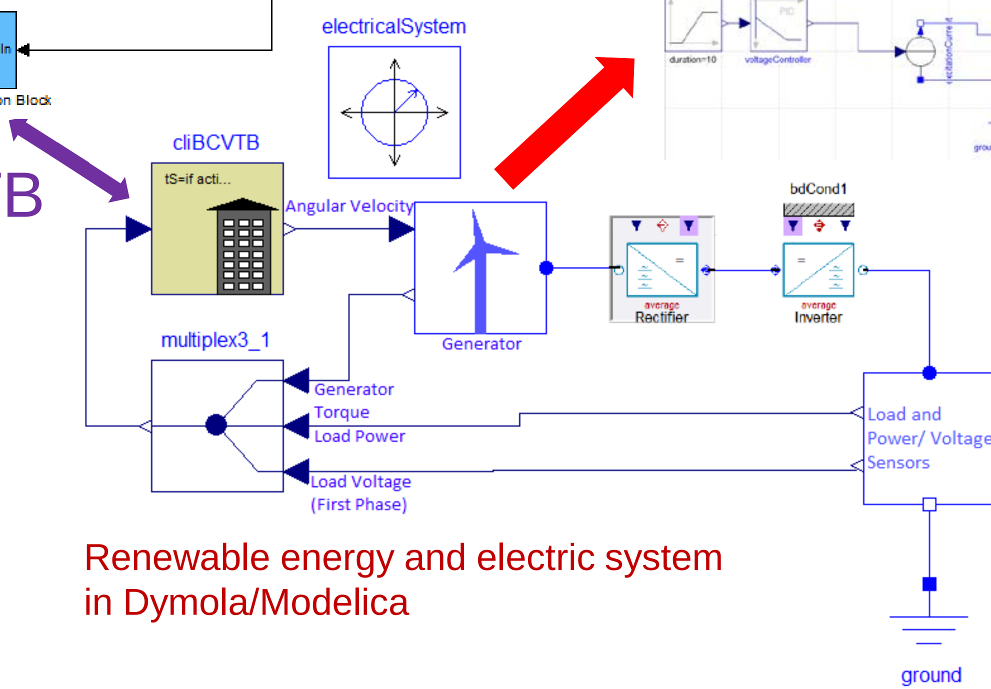
Generator with Voltage Controls



NREL's FAST Embedded in Simulink

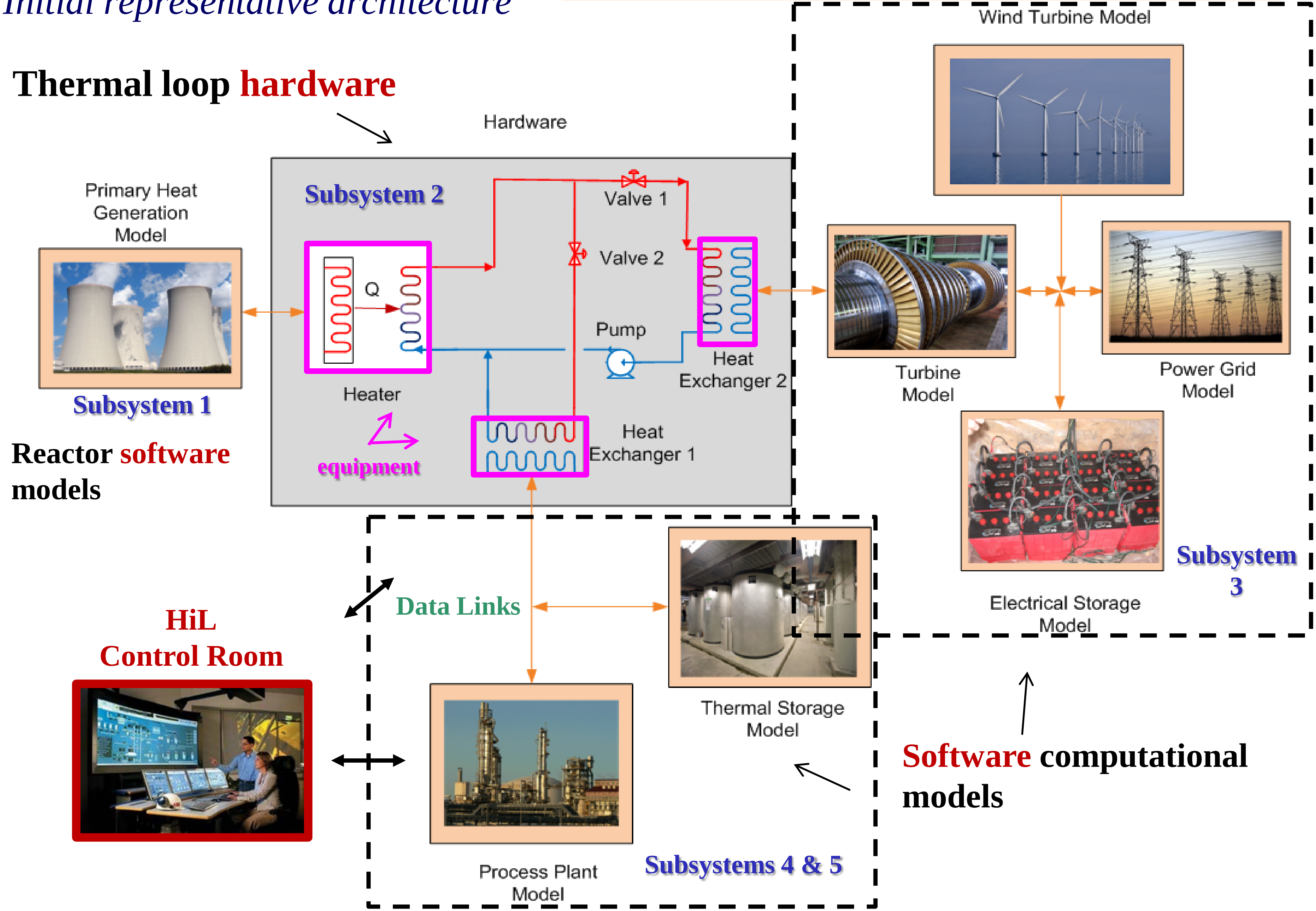


BCVTB



Renewable energy and electric system
in Dymola/Modelica

Configuration for HiL simulation of HES:
Initial representative architecture



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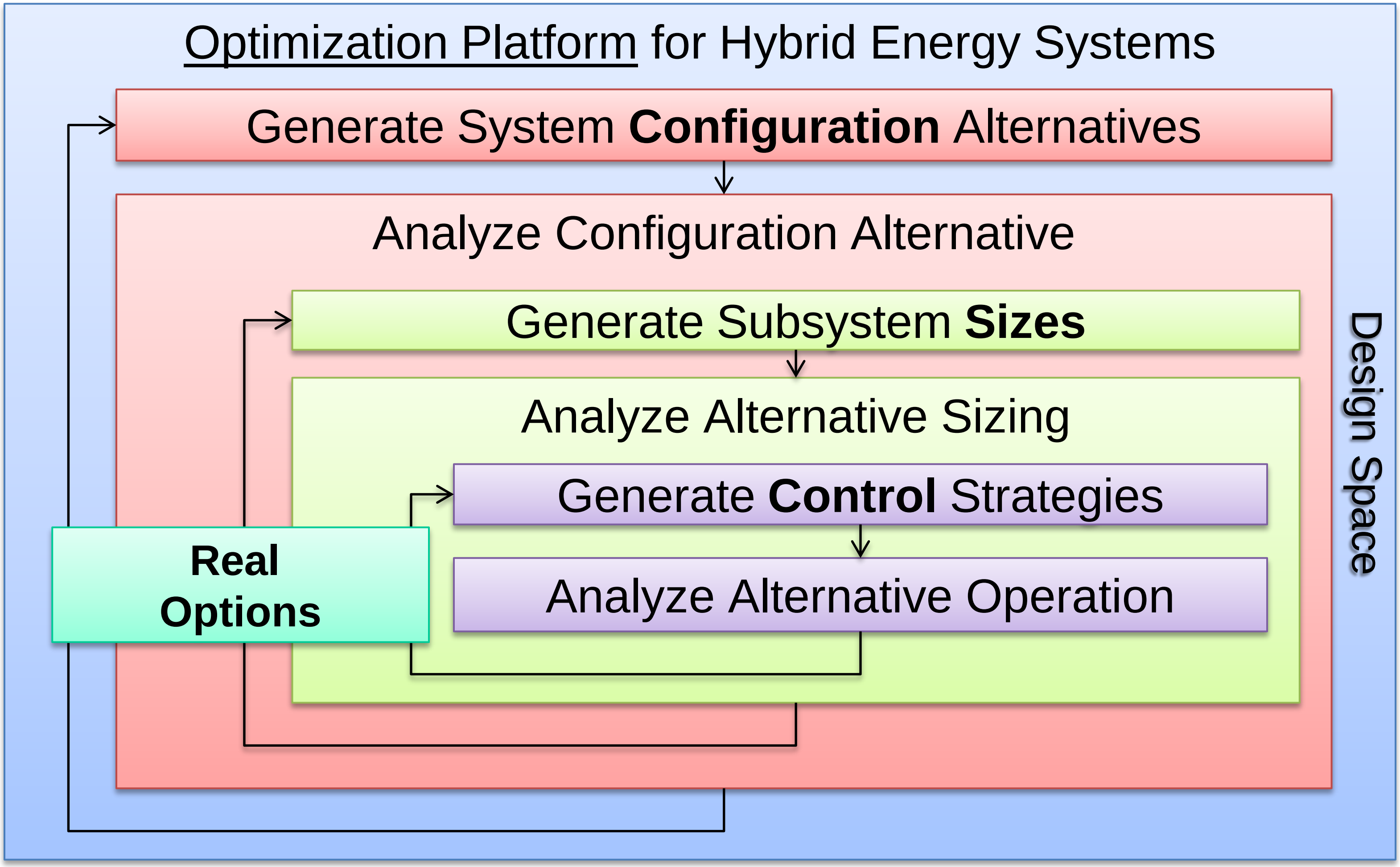
Optimization Challenge

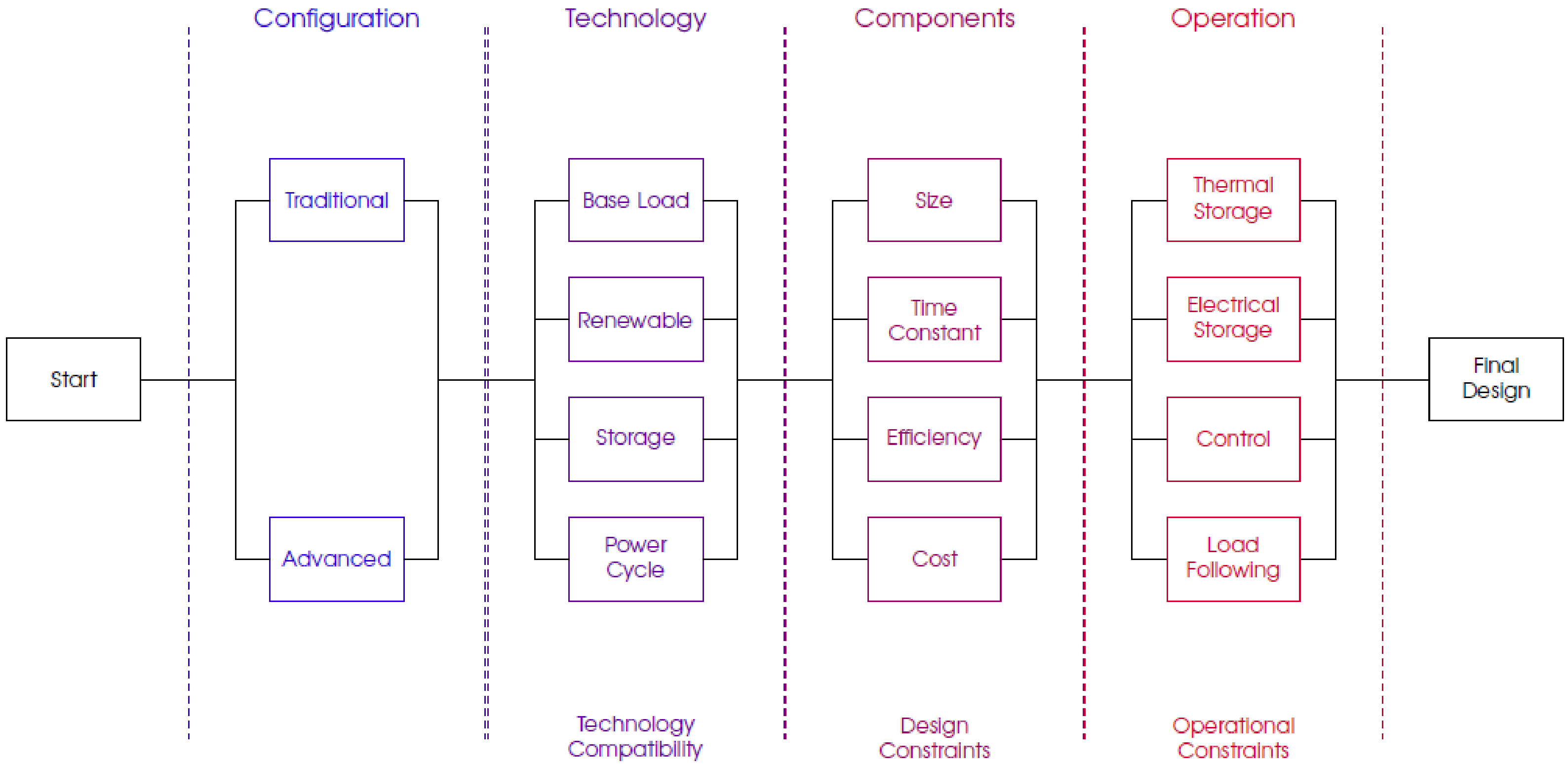


Optimizing one design variable without others does not guarantee an optimum and it is also inefficient and costly

Maximize Utility over Design Space: configuration, sizing, control, real options

Current Architecture

- Extending computational framework to consider:
  - more detailed models (physics-based);
  - alternative configurations and technologies;
  - operation and control of HES.
- A decision tree classifies design aspects into distinct layers:



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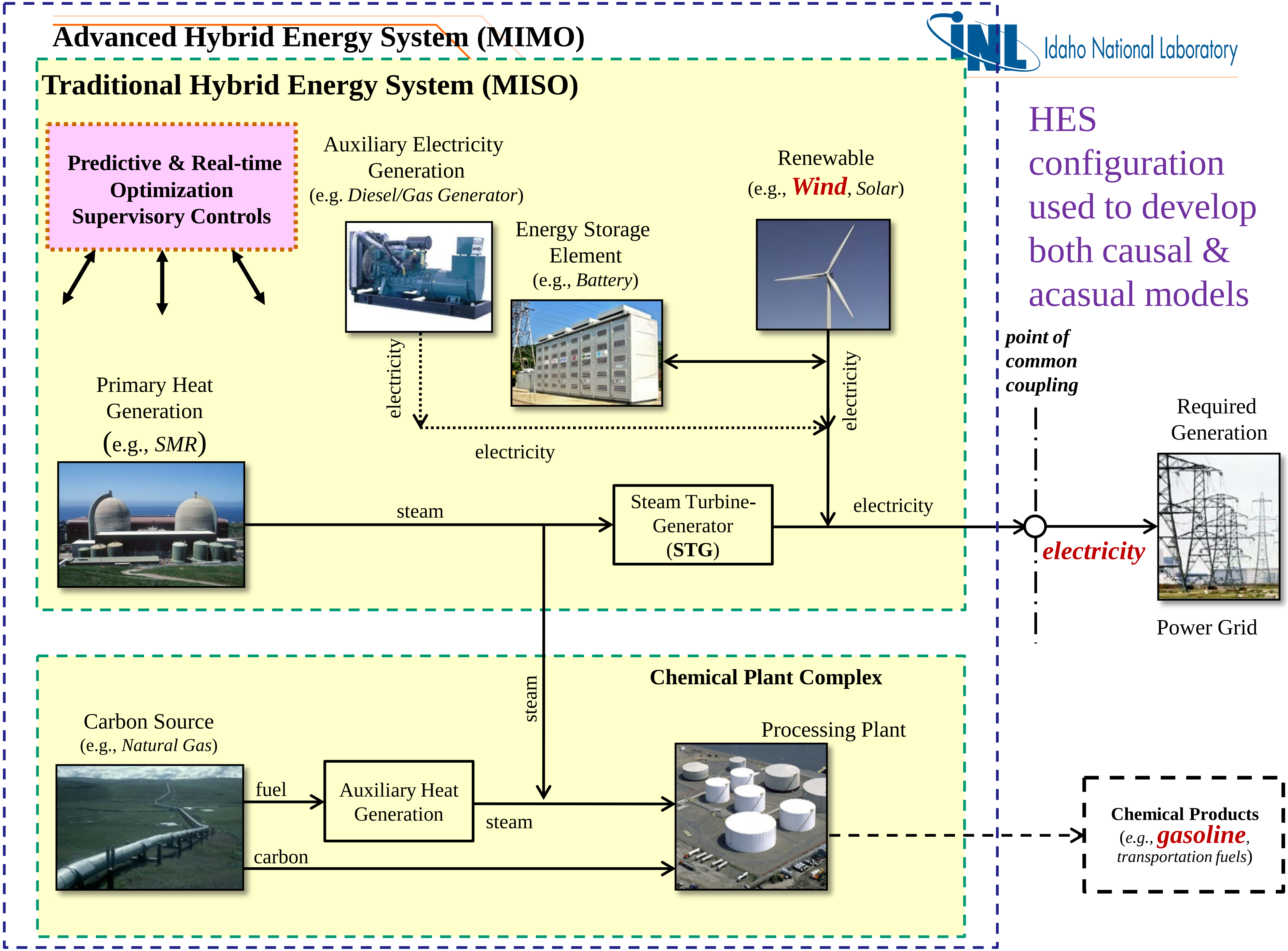
Advanced Hybrid Energy System (MIMO)
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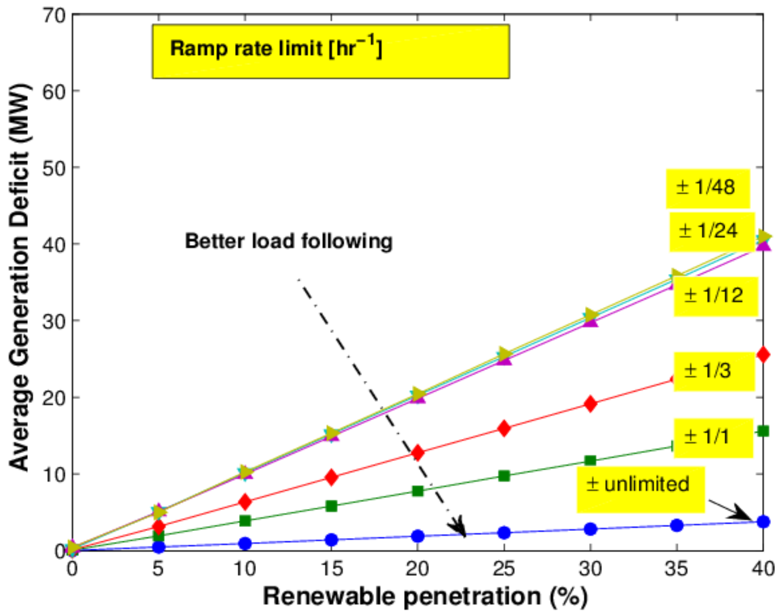
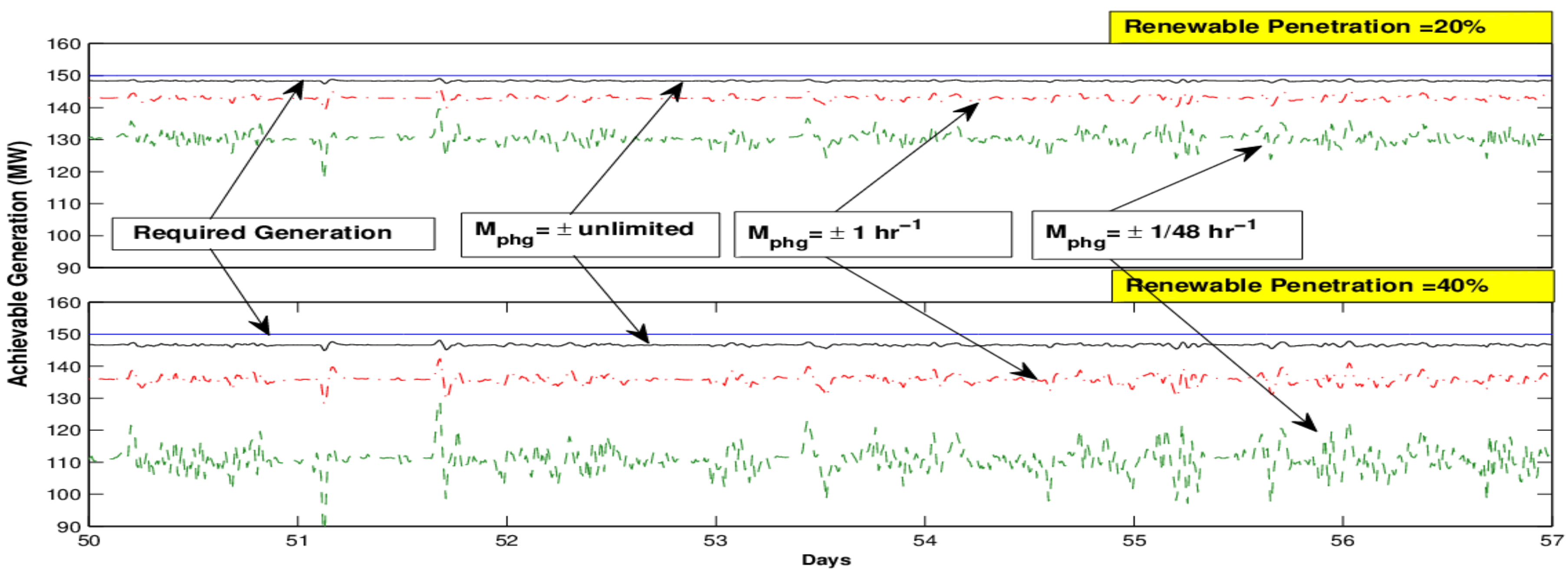
Traditional Hybrid Energy System (MISO)
Predictive & Real-time Optimization Supervisory Controls
Auxiliary Electricity Generation
(e.g. Diesel/Gas Generator)
Energy Storage Element
(e.g., Battery)
Renewable
(e.g., Wind, Solar)
HES configuration used to develop both causal & acasual models
electricity
electricity
electricity
Primary Heat Generation
(e.g., SMR)
steam
Steam Turbine-Generator (STG)
electricity
point of common coupling
Required Generation
electricity
Power Grid
Chemical Plant Complex
steam
Carbon Source
(e.g., Natural Gas)
fuel
Auxiliary Heat Generation
steam
Processing Plant
carbon
Chemical Products
(e.g., gasoline, transportation fuels)

Effect of primary heat generation maneuverability (load following) on achievable generation

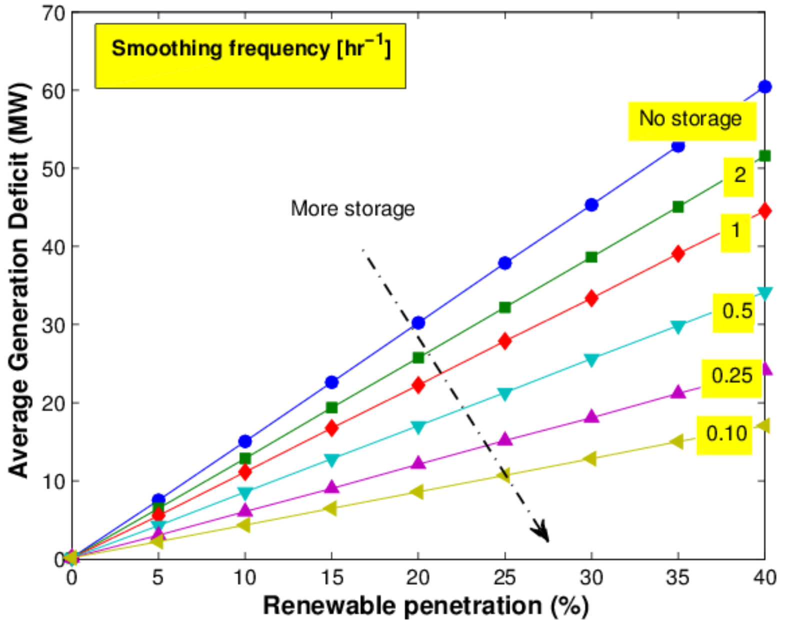


"Better load following facilitates achieving required generation"

Parameter: Maneuverability (load following) [hr^{-1}] of primary heat generation

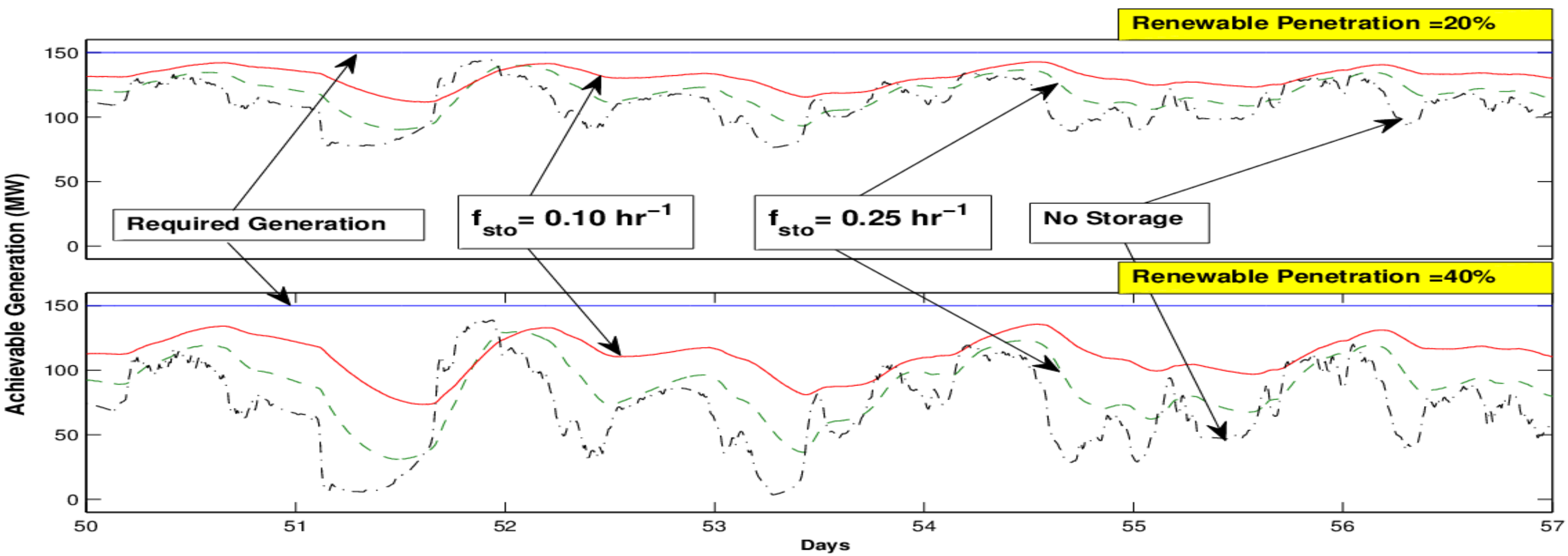


Effect of storage on achievable generation



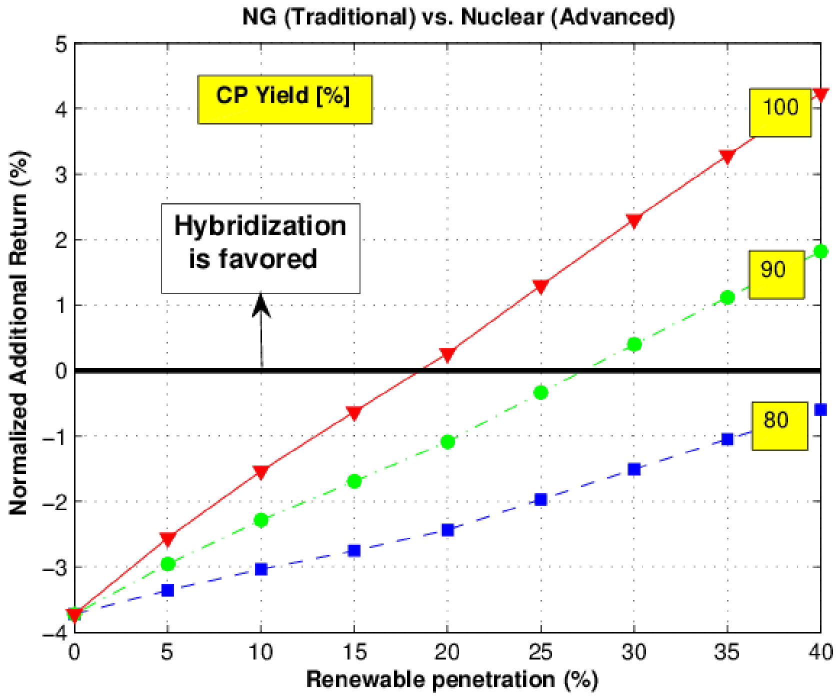
"More storage facilitates achieving required generation"

Parameter: smoothing of renewable variability due to storage [hr^{-1}]



Traditional (electricity-only) *NG-based HES vs. advanced* (electricity-methanol) *nuclear-based HES*

Relative profitability of advanced hybrid (MIMO) increases with increase in renewable penetration



An advanced nuclear hybrid becomes increasingly more economical than a traditional [electricity-generation-only] NG-based solution after 18% of renewable penetration

NG conversion to fuels is optimum use of resource including capital investment

$$NAR = \frac{(V_a - V_t)}{\hat{O}_a} \times 100$$

Subscript

t: traditional (*electricity*)

a: advanced (*electricity plus methanol*)

$$V = (R_e + R_{cp}) - (C_{cap} + C_{O\&M} + C_{var} + C_{env})$$

Assumption: $\hat{O}_{phg} = O_{phg} P_{phg}$

NAR:	Normalized Additional Return
V:	Value generated
R_e:	Revenues from electricity
R_{cp}:	Revenues from chemical products
C_{cap}:	Cost of capital
$C_{O\&M}$:	Cost of operations & maintenance
C_{var}:	Cost of variability
C_{env}:	Cost of environmental impact (CO_2 emission)
$\hat{O}$:	Adjusted overnight capital cost

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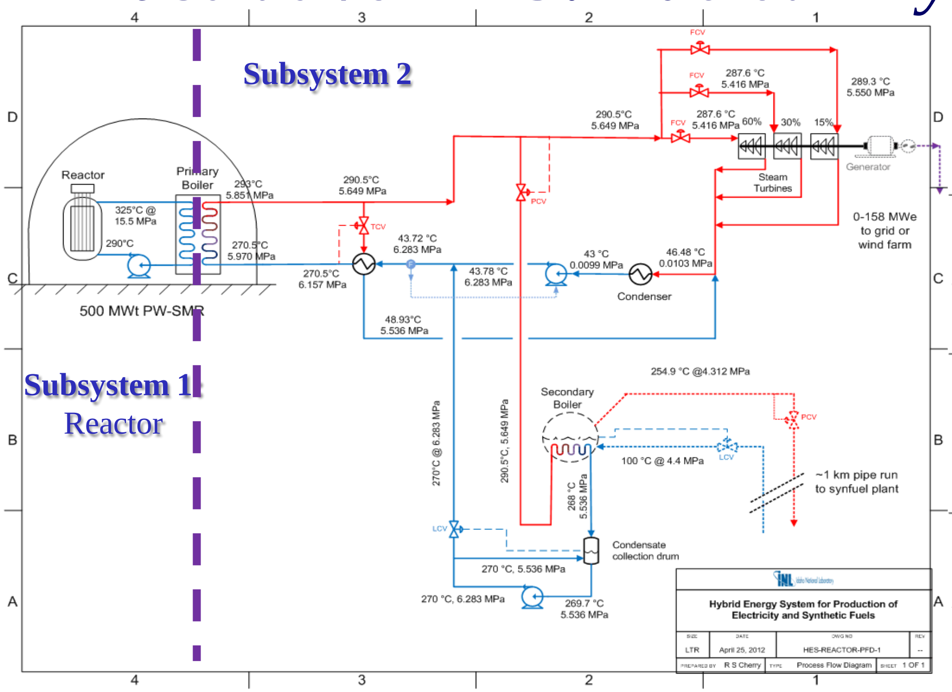
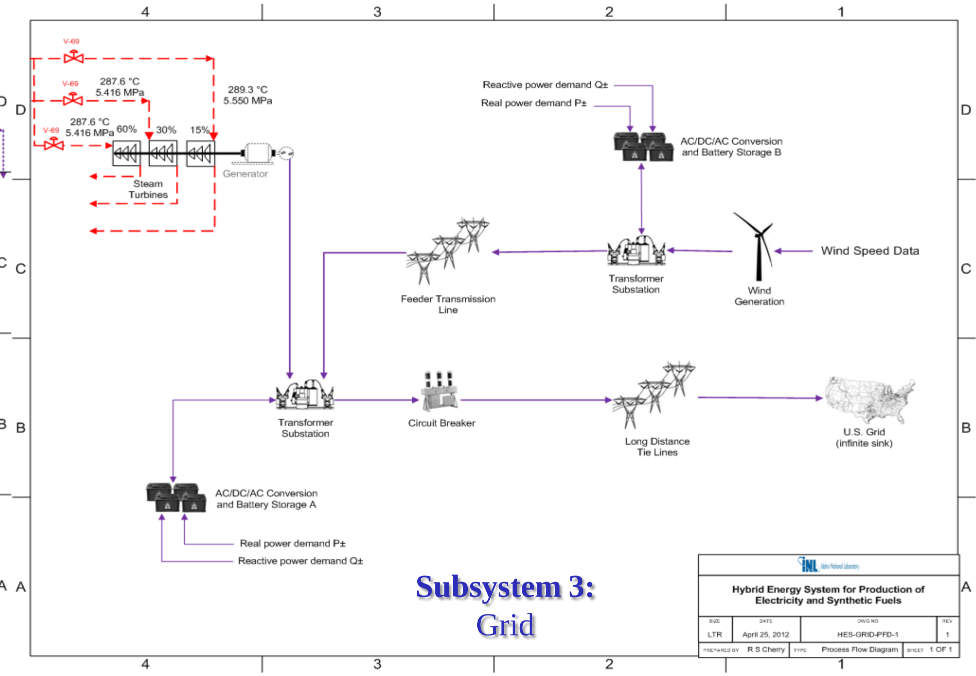
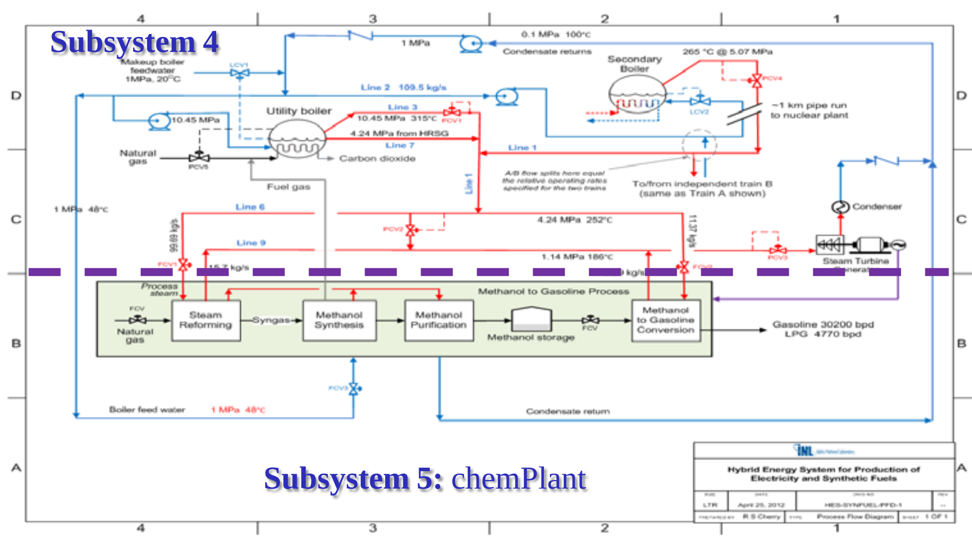
Illustrative HES: *Nuclear Hybrid w/ Renewables*





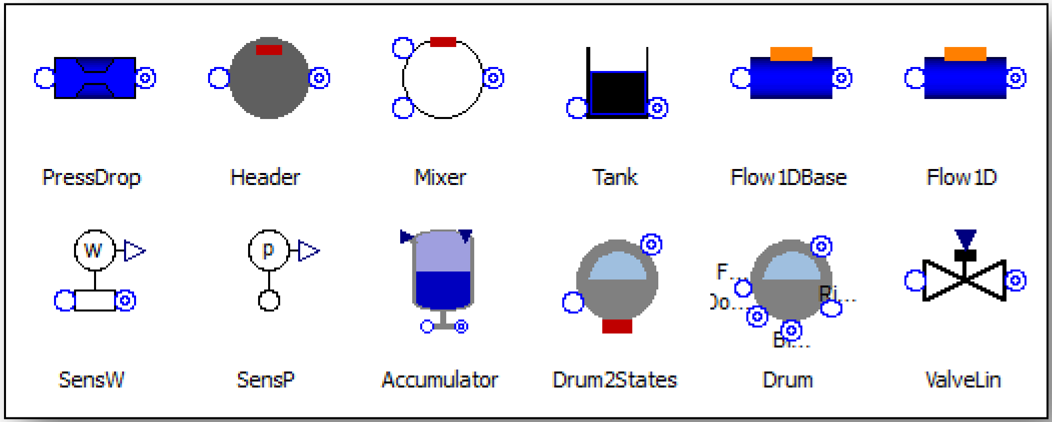
Predictive & Real-time Optimization Supervisory Controls

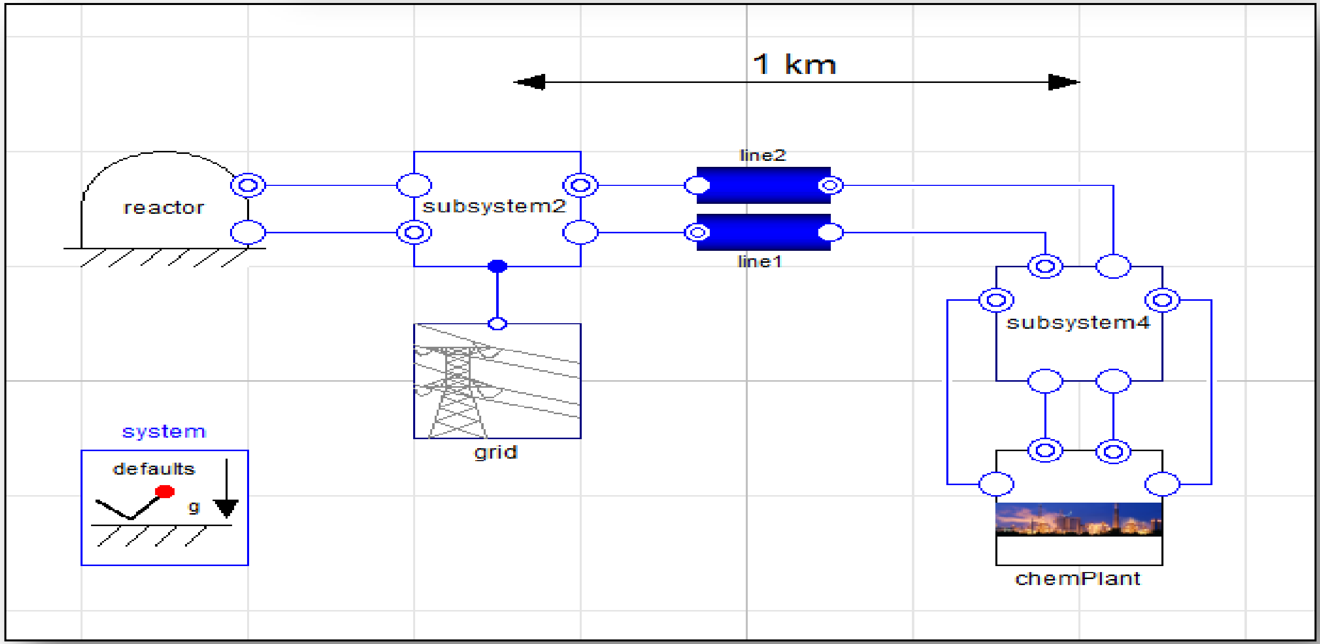


HES Computational M&S: Overview

- Builds on
  - In-house libraries
  - Open-source libraries

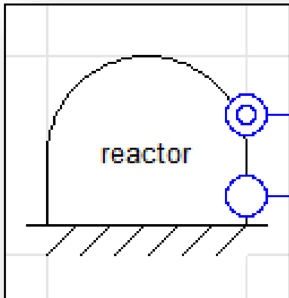
- Five main subsystems
  1. Reactor
  2. Power generation (subsys2)
  3. Electrical grid
  4. Steam control (subsys4)
  5. Chemical plant



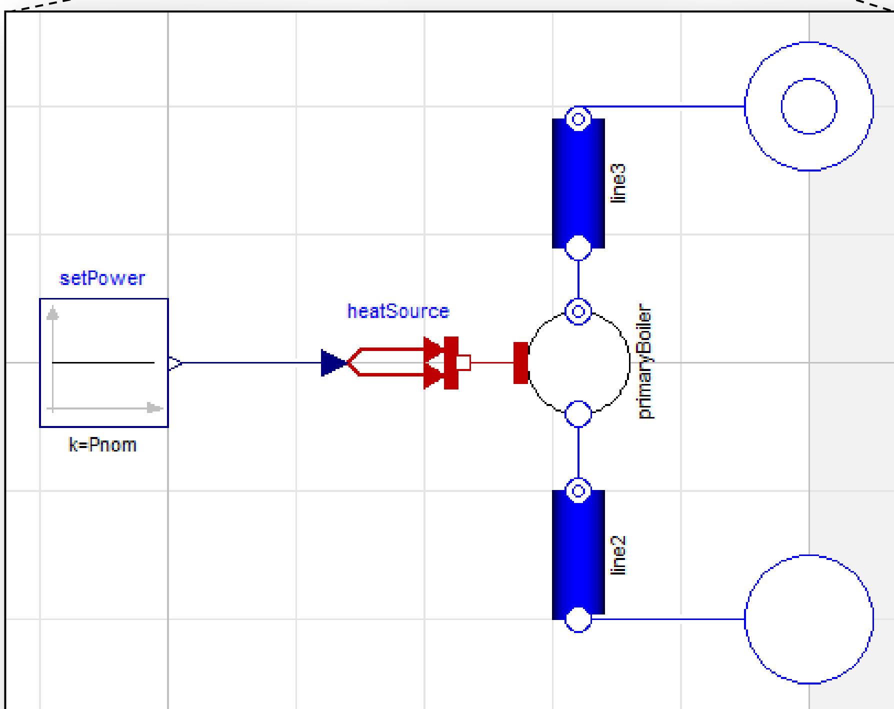


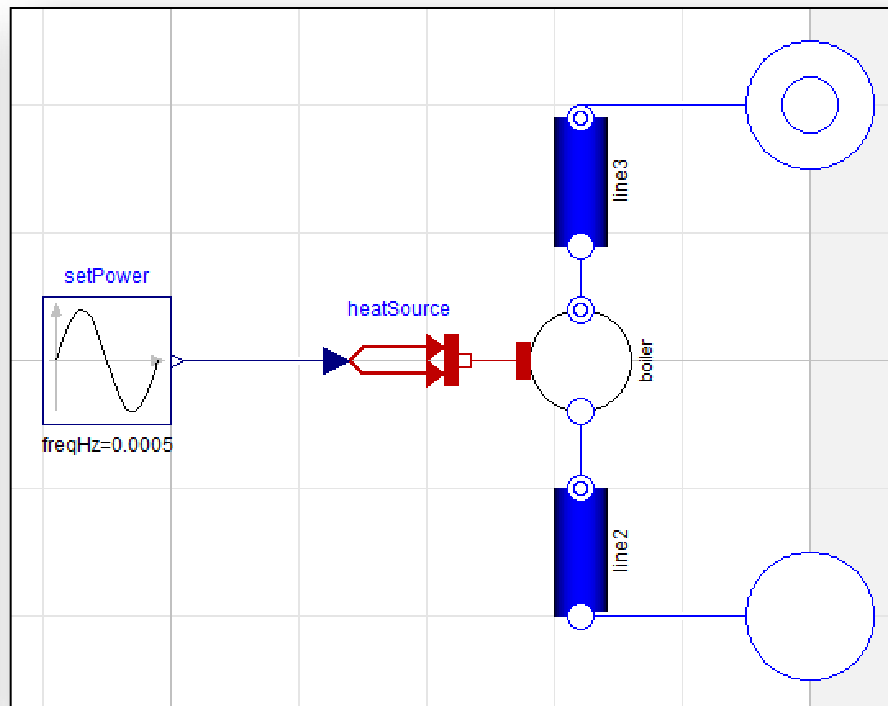
Reactor

- Reactor



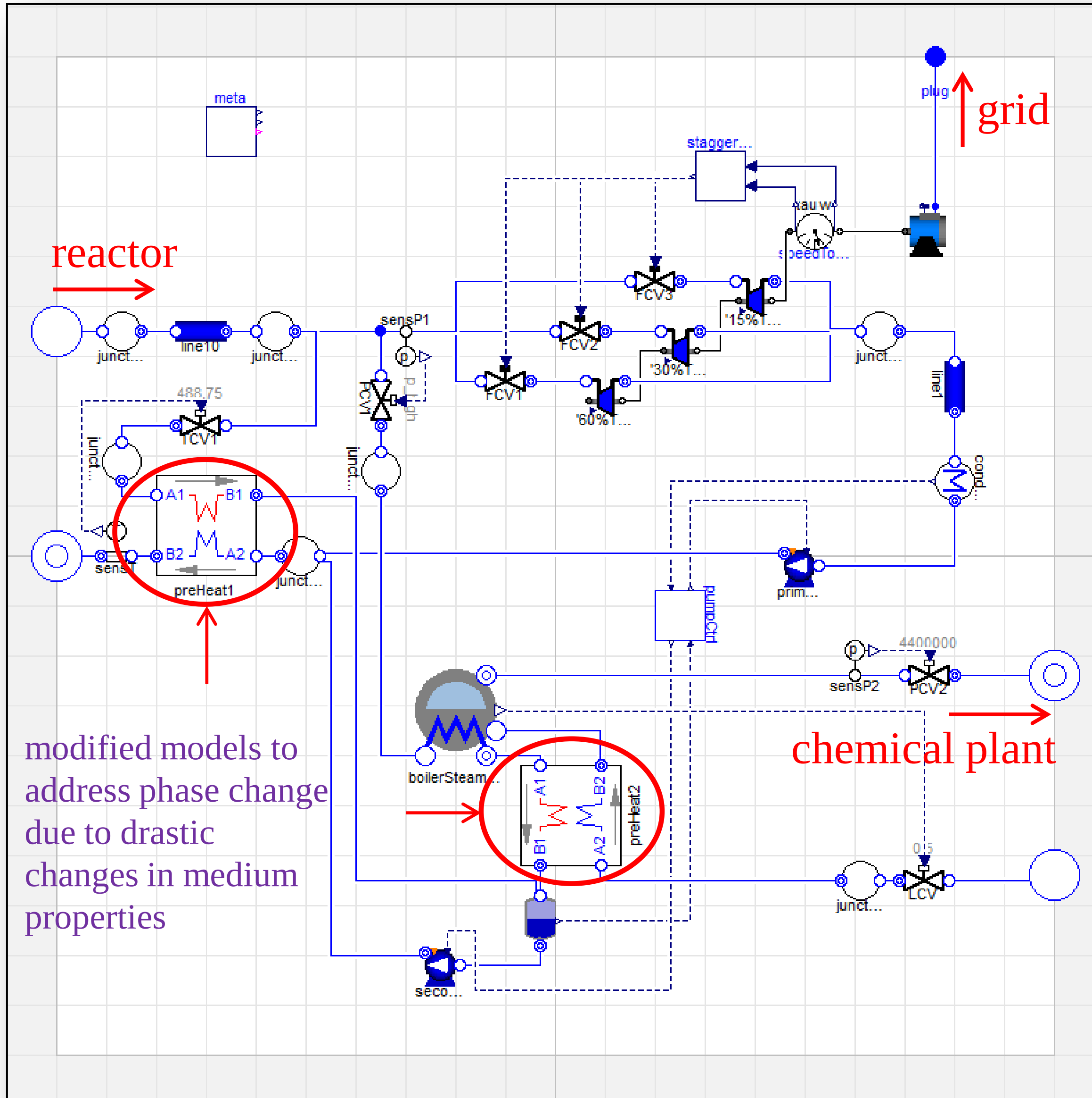
- Constant heat source
- Next: exploring partial load-following





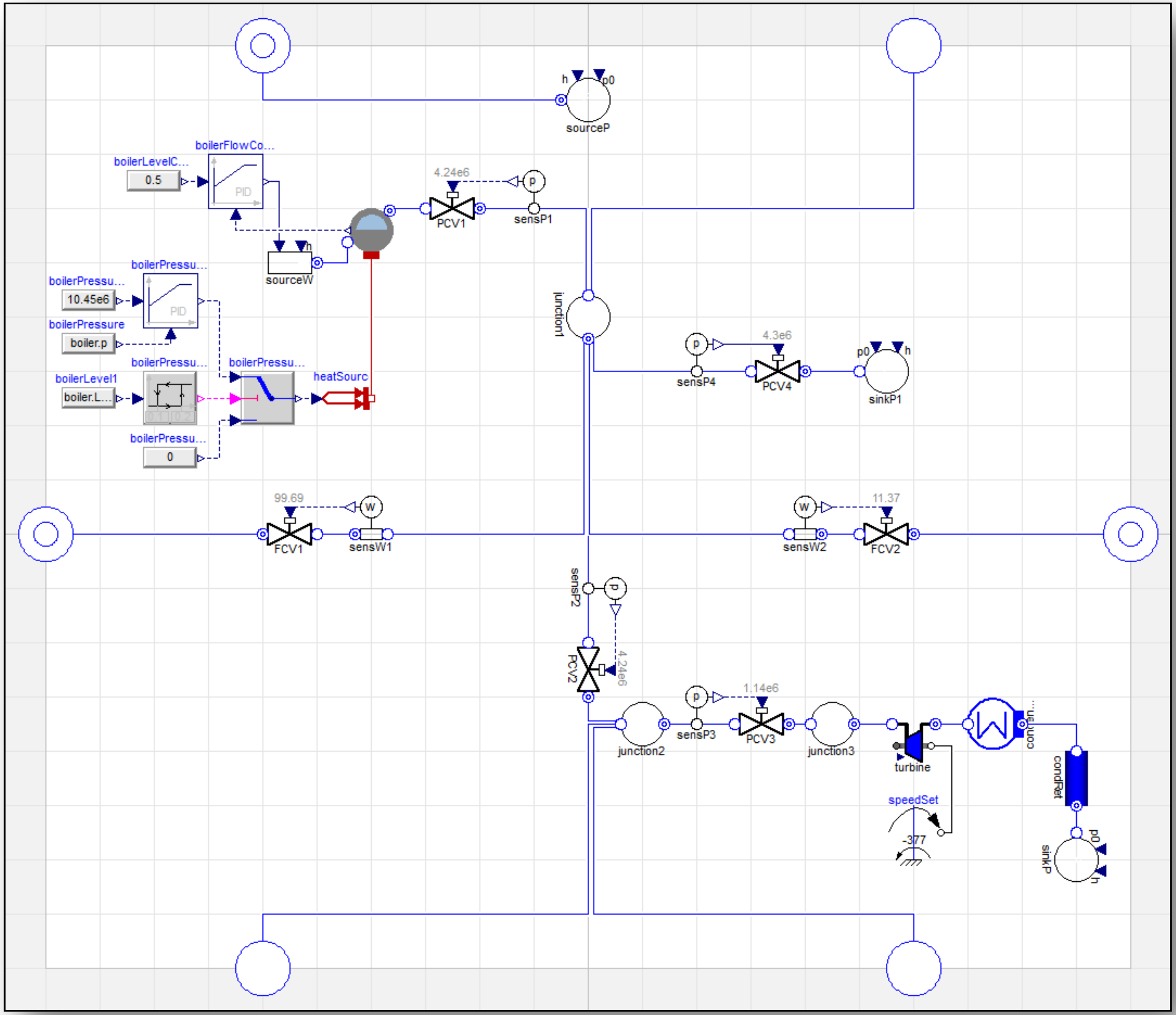
Power Subsystem

- Two loops
  - Three turbines
  - Secondary boiler
- Turbines have priority
  - 3 coaxial turbines
  - Sized as 60%, 30%, 15% of nominal
- Coordinated two-pump control
  - Maintain 311°C at reactor outlet by varying flow rates



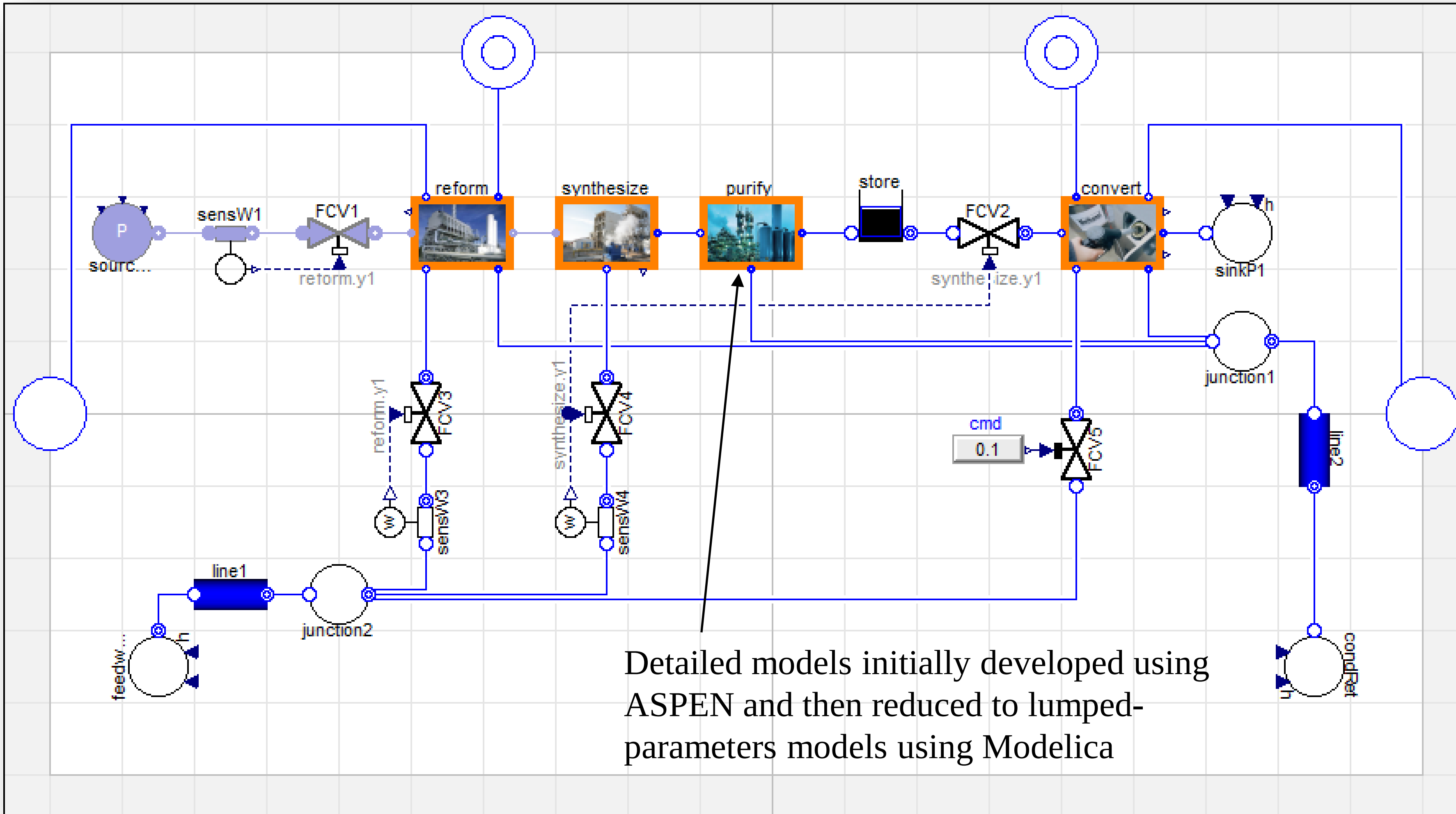
Power Control for Chemical Plant

- Low-pressure and high-pressure steam headers
- Utility boiler compensates for variation in steam coming from Power Subsystem
- Waste heat recovered in secondary turbines



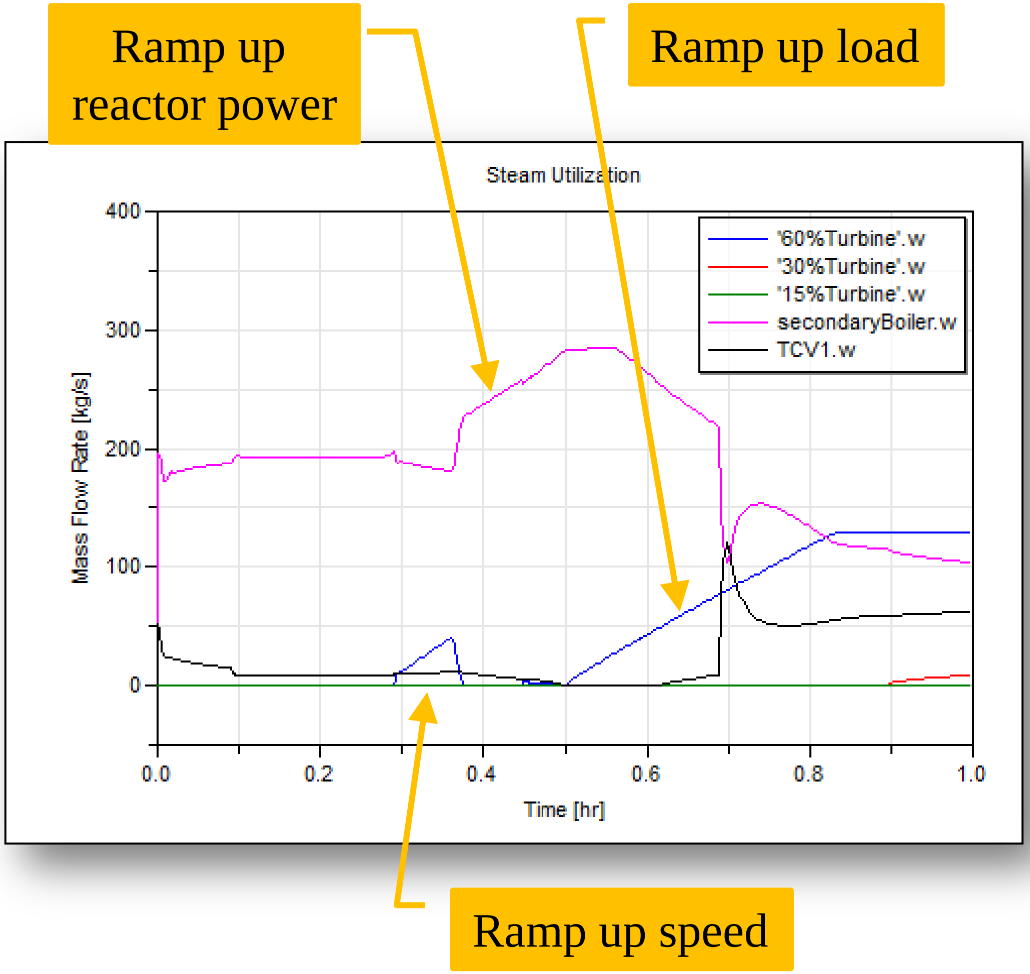
Chemical Plant

- Process-based reduced-order models (ROM)



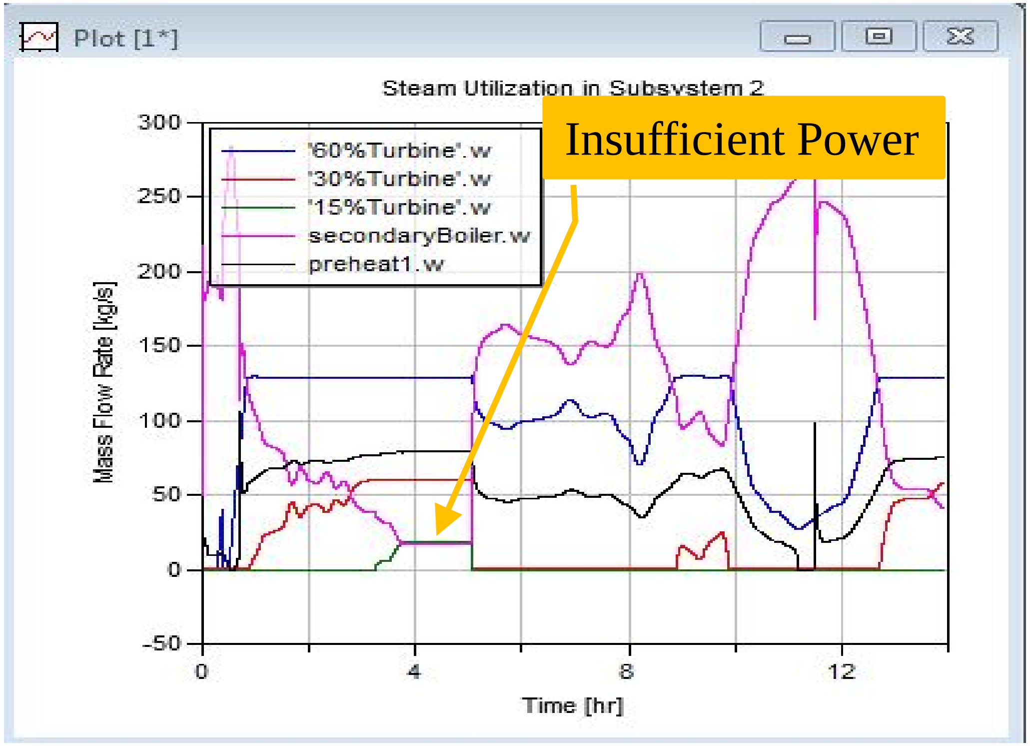
Power Subsystem Start-up / Shutdown

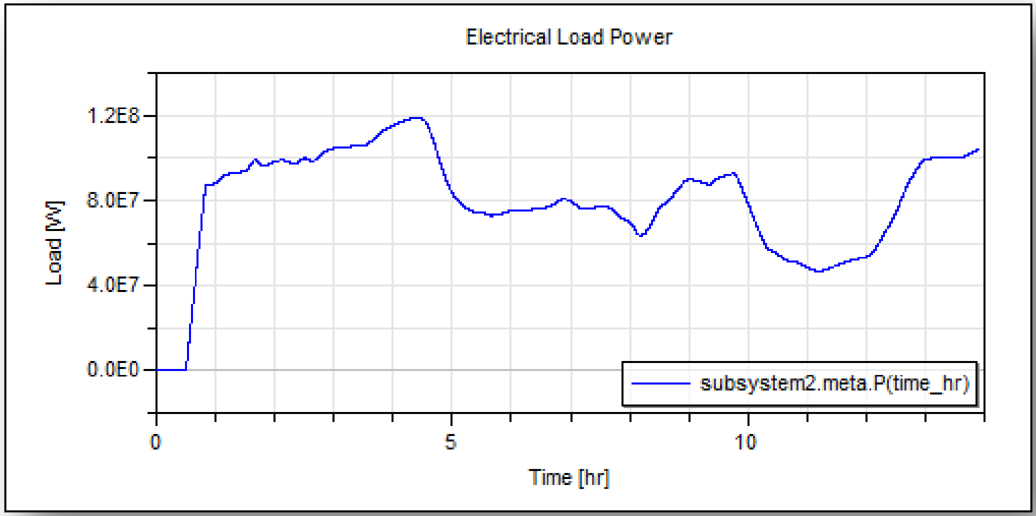
- Three P, T (h)
  - Reactor inlet
  - Reactor outlet
  - Condenser inlet
- Nominal RPM for both pumps
- Startup sequence
  - Start turbines idle at 0 RPM
  - Wait for transients to die out
  - Ramp up turbine to 60Hz
  - Ramp up reactor power
  - Ramp up load to nominal at 60Hz



Compensating for Variation in Wind Power

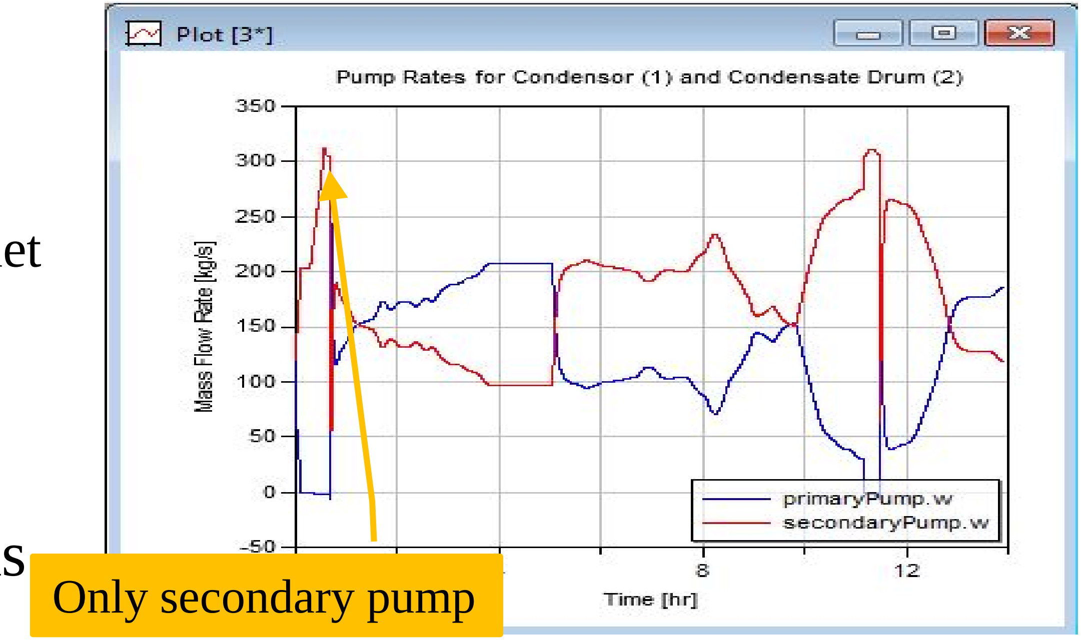
- Three turbines turn on or off to produce desired electrical power
- Insufficient power could be covered using grid-battery
- Excess steam is diverted to secondary boiler and on to chemical plant

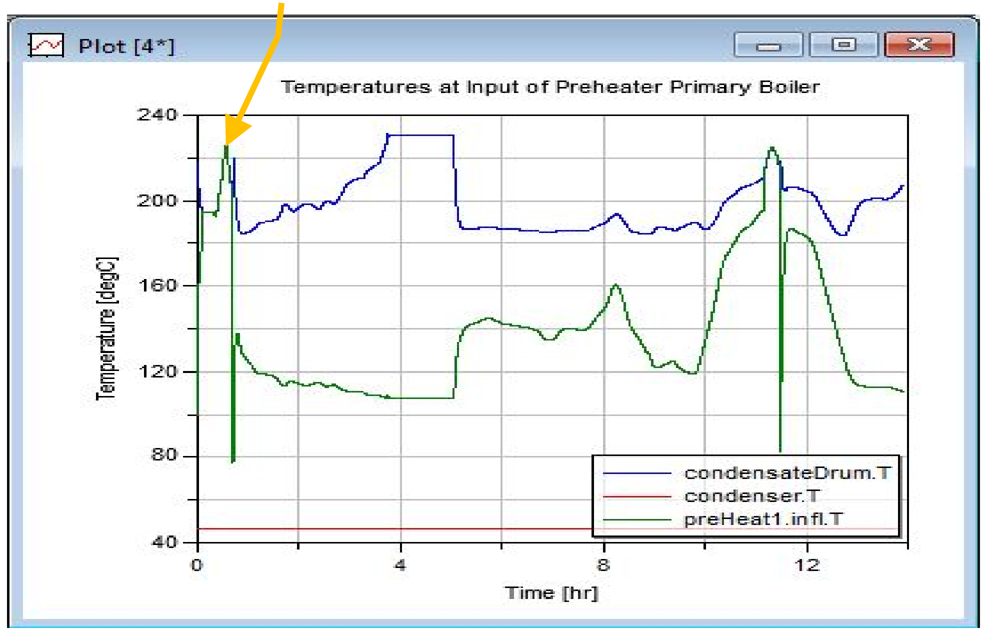




Controlling the Pumps

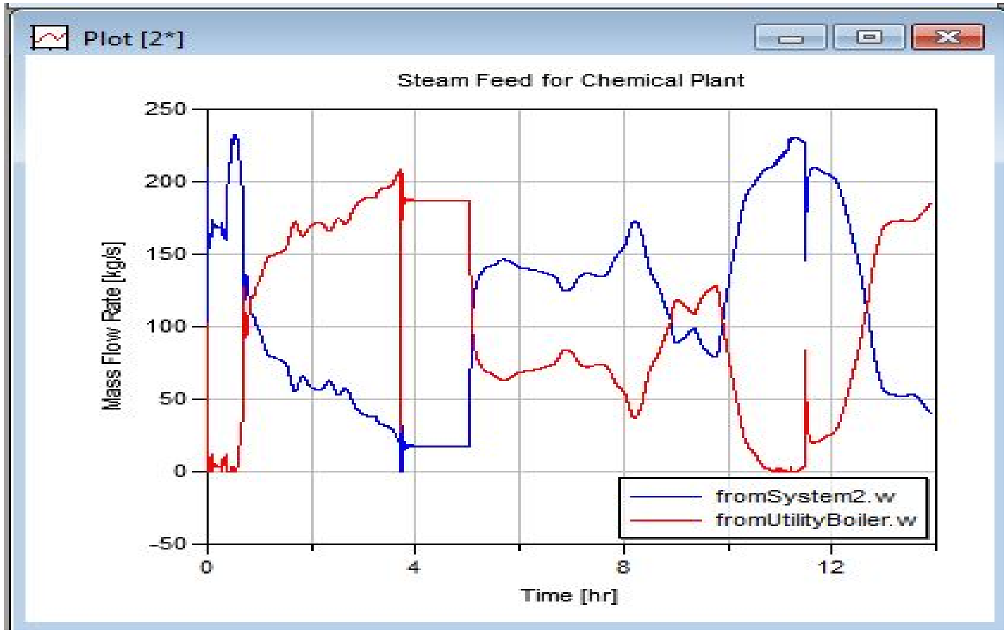
- Coordinated pump control
  - Maintain 311ºC at reactor outlet by varying flow rates
- Variable speed pump control
- Total mass flow divided proportional to level of drums
- Temperature of the input flow to pre-heater of primary boiler varies significantly depending on which pump the feed comes from

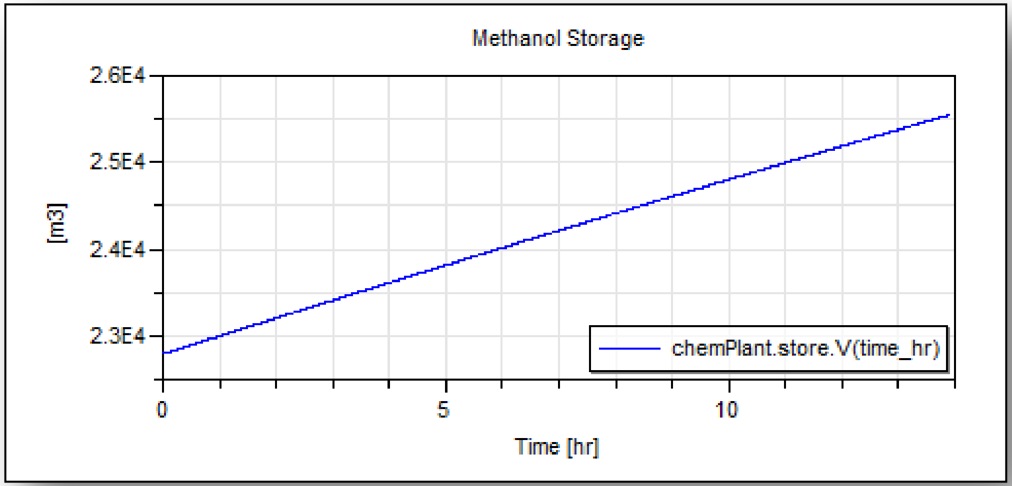




Chemical Plant

- Utility boiler compensates for variation in steam coming from Power Subsystem
- Chemical plant currently runs in steady state
- Methanol stored increases at constant rate





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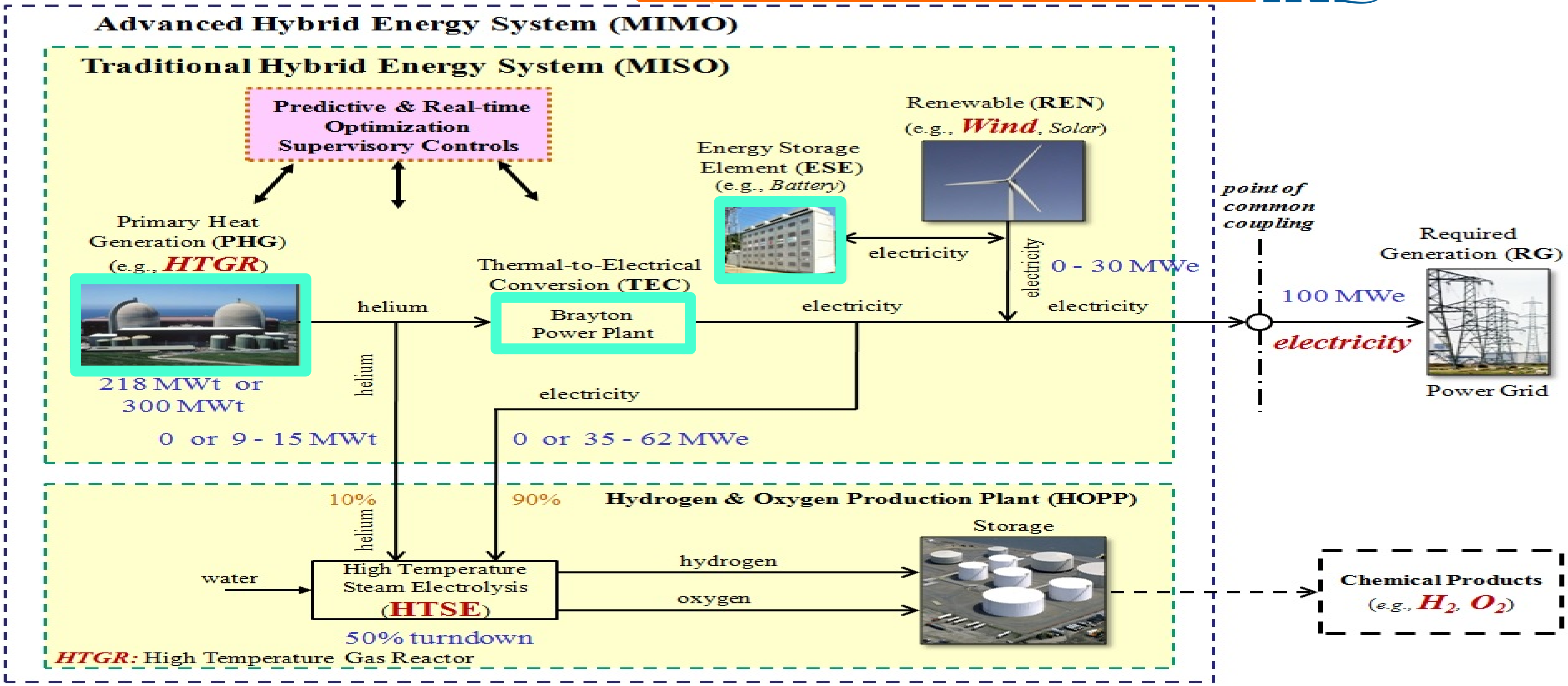
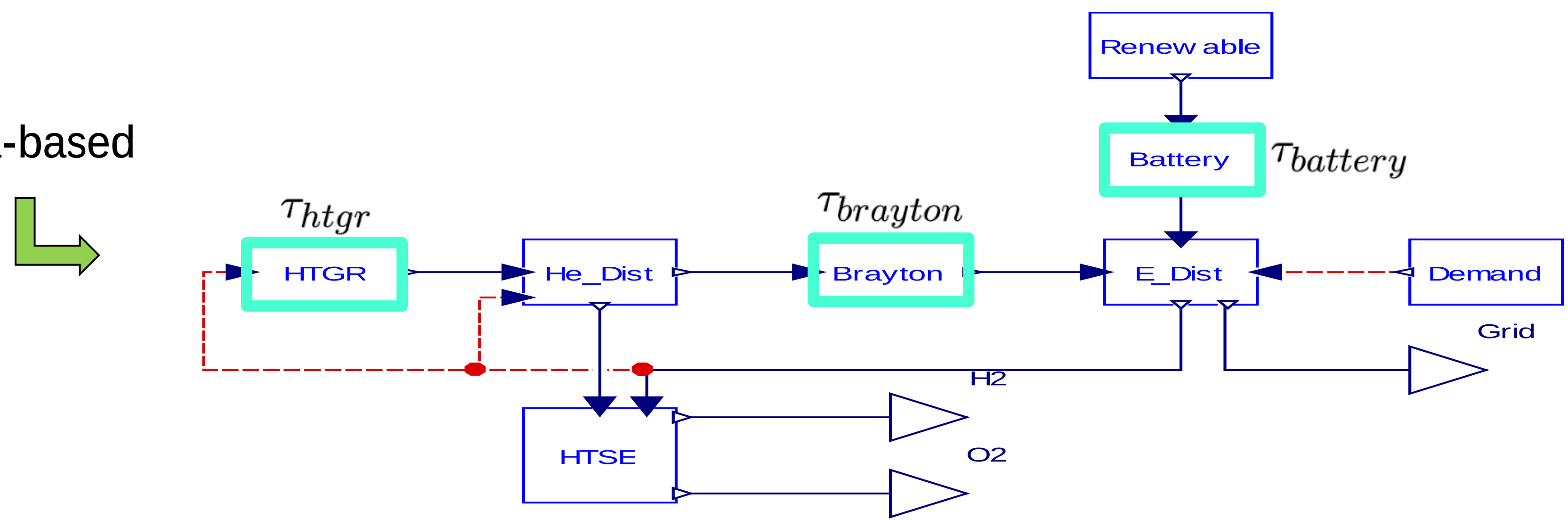
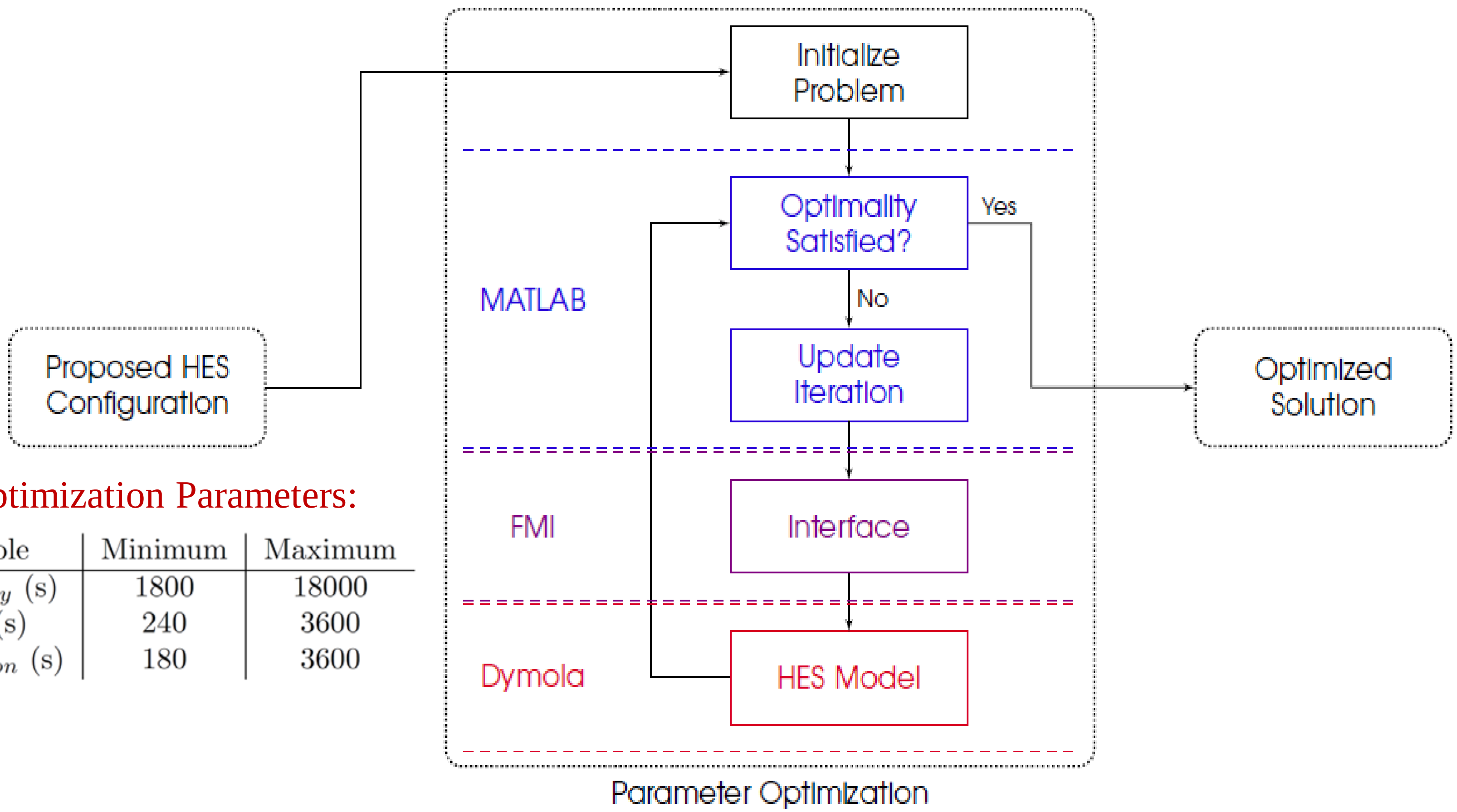


Modelica-based Model



Computational Framework

- Three major software tools comprise the present framework:
  - Dymola – platform for Modelica-base HES model;
  - MATLAB – platform for numerical optimizer;
  - FMI – interface for Dymola and MATLAB to execute HES simulations.



Optimization Parameters:

Variable	Minimum	Maximum
$\tau_{battery}$ (s)	1800	18000
τ_{htgr} (s)	240	3600
$\tau_{brayton}$ (s)	180	3600

Optimization Methodology

- General optimization problem minimizes objective function for certain constraints:

$$\text{minimize } f(x), f: \Re^n \to \Re$$
$$\text{subject to} \begin{cases} x_{lower} \leq x \leq x_{upper} \\ c_k(x) \leq 0, k = 1, \dots, m \\ \hat{c}_j(x) = 0, j = 1, \dots, \widehat{m} \end{cases}$$

- Many optimizers for solving this problem exist; we use the Nelder-Mead simplex method (gradient-free thus suitable for noisy functions).

- Objective function is defined as the total variability in HTSE electrical power $P^e_{htse}(t)$:

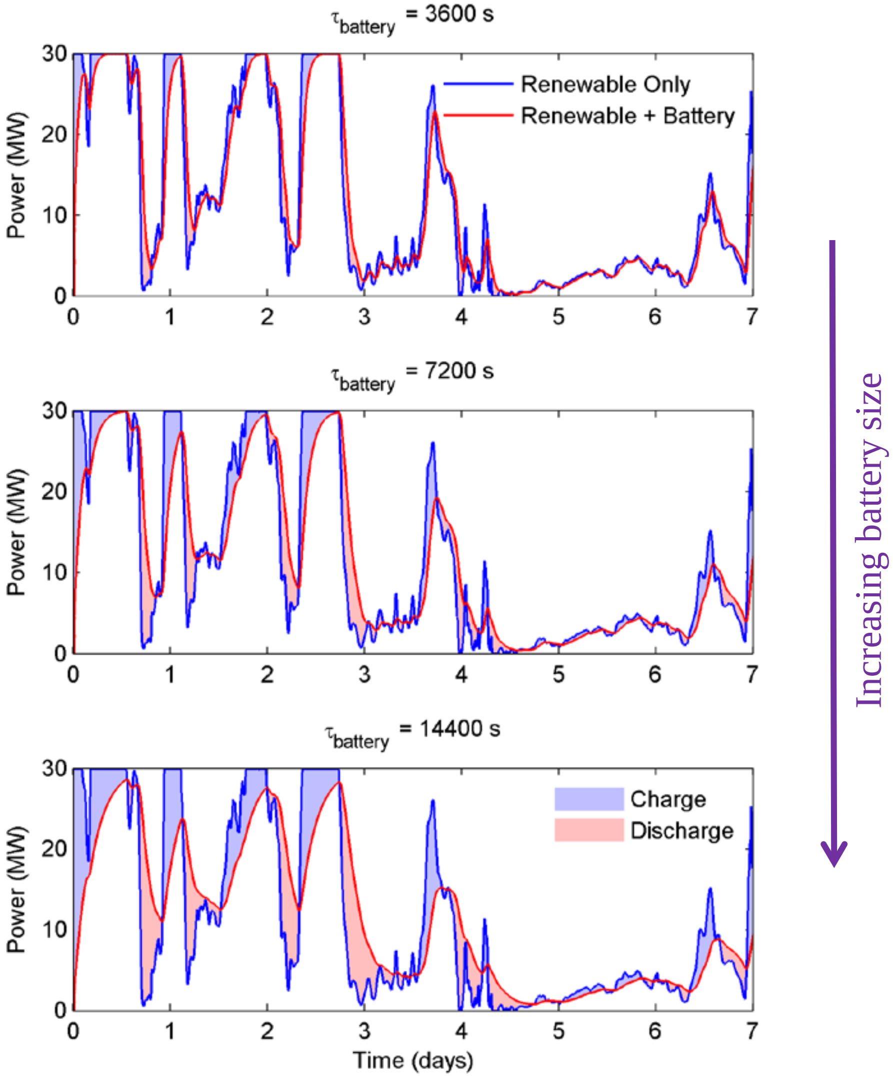
$$f(x) = \int_0^{t_f} |P^e_{htse}(t) - \bar{P}^e_{htse}|dt$$

- Constraints are enforced by modifying objective function with a quadratic penalty function:

$$\varphi(x) = f(x) + p(x) = f(x) + \sum_{i=1}^{m+\widehat{m}} b_i \max(0, c_i)^2$$

Effect of Battery Size

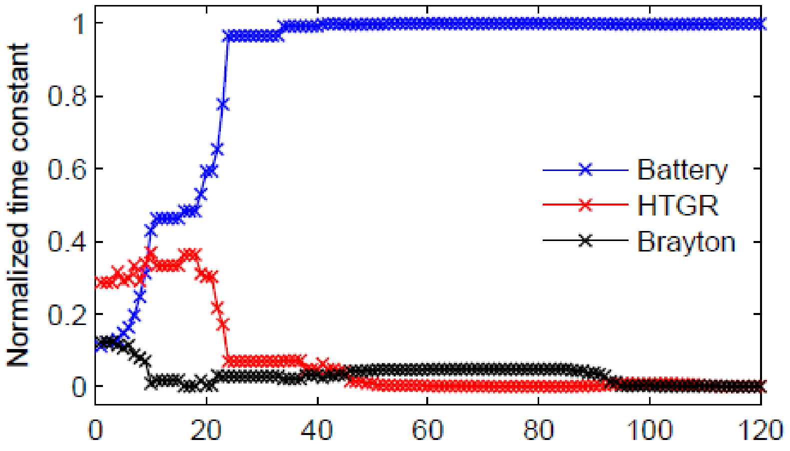
- Shaded area is electrical energy storage associated with the battery.
- Battery sizing and operation is a complex problem involving competing objectives
  - less battery storage leads to greater electrical variability (leading to higher operational cost of the system);
  - more battery storage smoothes out electrical variability from renewables (leading to higher capital cost of the system).

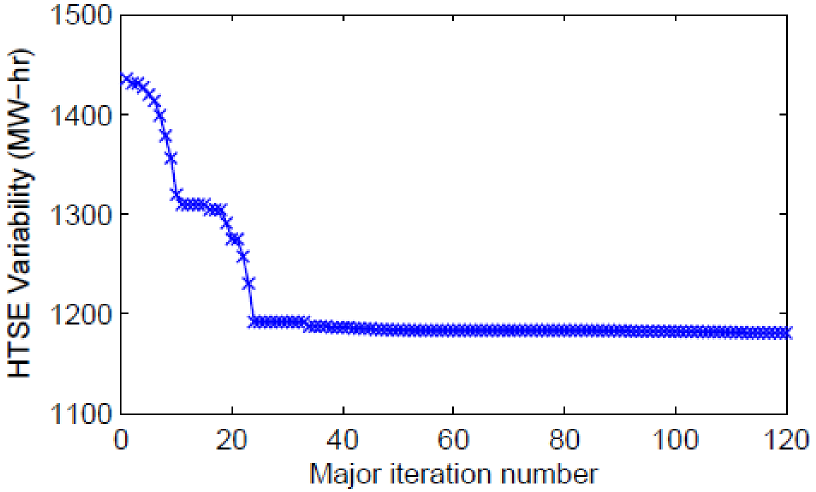


Unconstrained Optimization Results

- Without constraints, time constants converge to bounds:
  - larger battery ($\tau_{battery}$ = 18000 s) smoothes out renewable variability;
  - fastest reactor (τ_{htgr} = 240 s) and power cycle ($\tau_{brayton}$ = 180 s) aid in load following.
- Constraints need to be included to properly account for negative impacts of larger battery and faster reactor/power cycle (i.e., higher cost).
- Time constants normalized based on upper and lower bounds:

$$\tau^* = \frac{\tau - \tau_{\min}}{\tau_{\max} - \tau_{\min}}$$





Constrained Optimization Results

- Linear cost function used as inequality constraint:

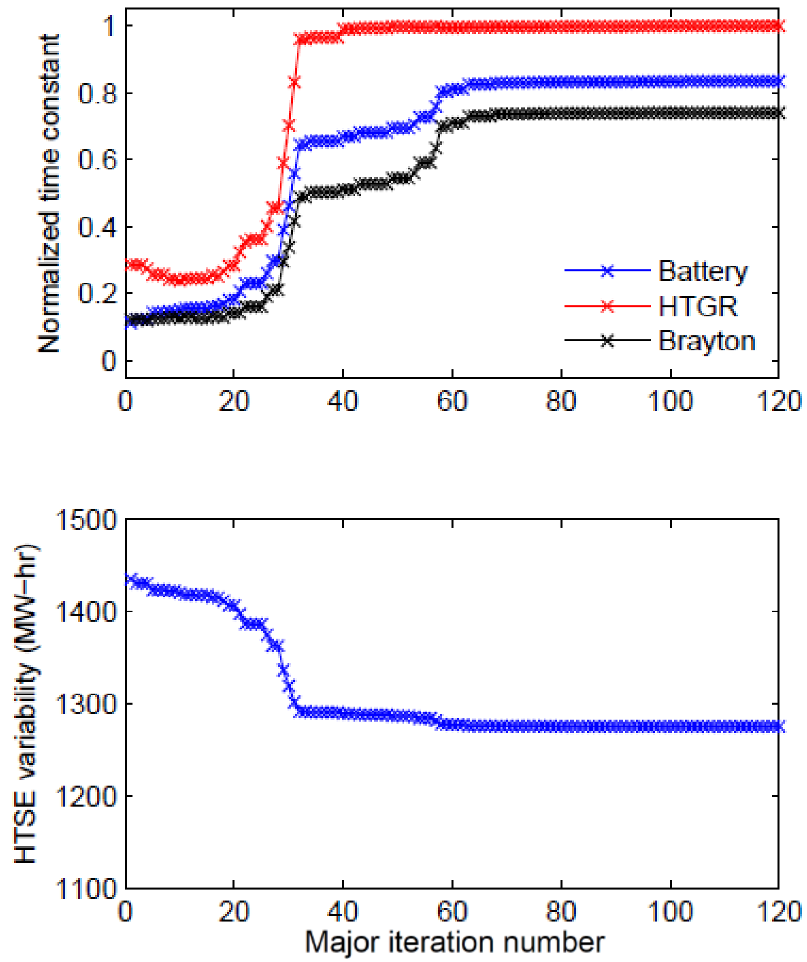
$$c_1(x) = k_1\tau_{battery} - k_2\tau_{htgr} - k_3\tau_{brayton} \leq 0$$

- Two nonlinear constraints restrict the relative time constants of HTGR and Brayton cycle:

$$c_2 = \frac{\tau_{htgr}}{\tau_{brayton}} - 2 \leq 0$$

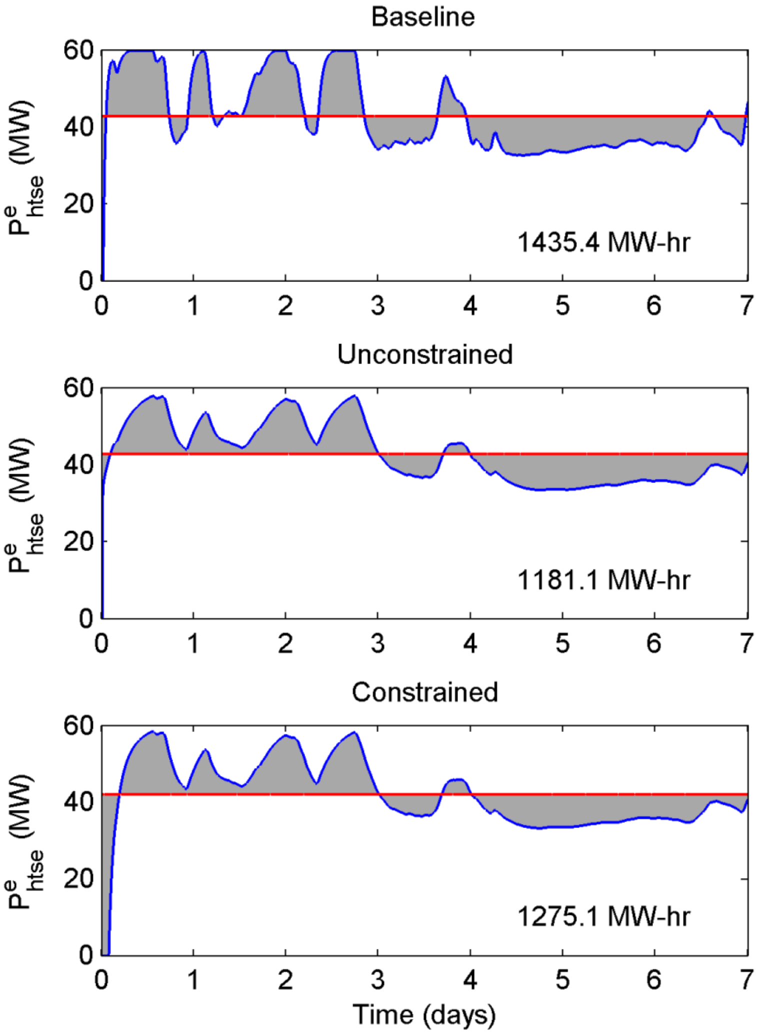
$$c_3 = \frac{\tau_{brayton}}{\tau_{htgr}} - 2 \leq 0$$

- Constraint forces optimizer to compromise between competing effects of performance and cost.
- One time constant converges to the maximum value (HTGR); others to optimal intermediate values



Optimization Summary

	Baseline	Unconstrained	Constrained
$\tau_{battery}$ (s)	3600	18000	15311
τ_{htgr} (s)	1200	240	3600
$\tau_{brayton}$ (s)	600	180	2712
$f(x)$ (MW-hr)	1435.4	1181.1	1275.1



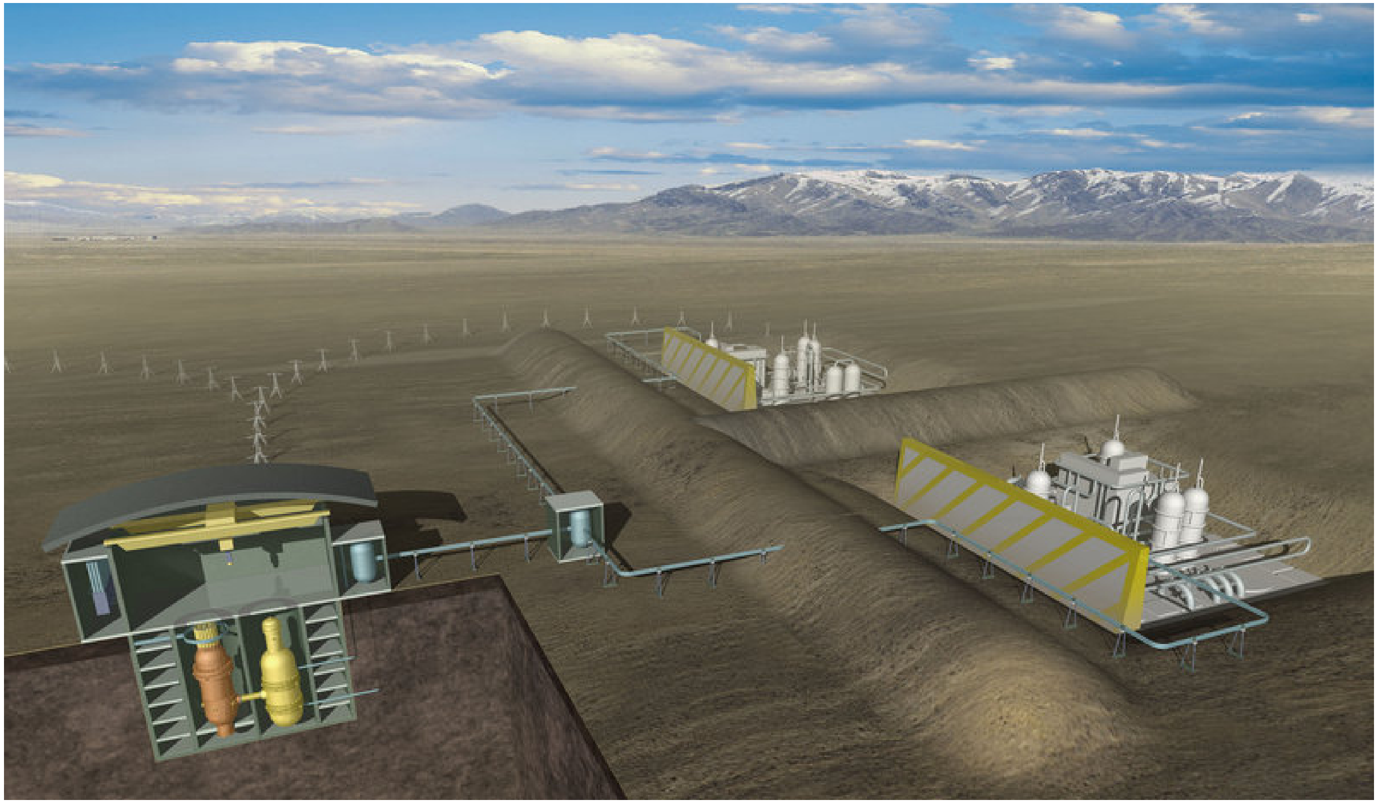
- Variability in HTSE electrical power is reduced by 18% and 11% using unconstrained and constrained optimization, respectively.
- Shaded area graphically illustrates effect of dynamic optimization:
  - HTSE operation is smoothed out to reduce variability;
  - primary effect of constraints is slower initial ramping of HTSE;

Variable	Minimum	Maximum
$\tau_{battery}$ (s)	1800	18000
τ_{htgr} (s)	240	3600
$\tau_{brayton}$ (s)	180	3600

Conclusions & On-going Directions

- Complex dynamics occur due to:
  - transient physical behavior, controller interactions, renewables variability & uncertainty
- Cannot be adequately analyzed using steady-state tools (e.g., in Aspen)
- Dynamic M&S crucial for design and operation of Hybrid Energy Systems
- Development of additional M&S capabilities
  - RTDS & hardware co-simulation connectivity
  - wind / solar application models
  - chemical process models (e.g., high temperature steam electrolysis, HTSE)
  - SMR models
  - Robust models for predicting anomalous operating conditions
- Development of design optimization techniques, tools & technologies
- Development of hardware capabilities (e.g., thermal loop for HiL demo)
- Development of predictive (look-ahead) supervisory controls & real-time optimization for optimized operations and economics
- Detailed analysis of dynamics of tightly-coupled power generation -process systems and design of systems to moderate the extremes
- …

Questions ?



Conceptual nuclear-driven complex for power, hydrogen, and synfuel production