Techno-Economic Optimization of Advanced Energy Plants with Integrated Thermal, Mechanical, and Electro-Chemical Storage

Award#:DE-FE0031771

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2021 University Turbine Systems Research Project Review Meeting November 9, 2021







Outline

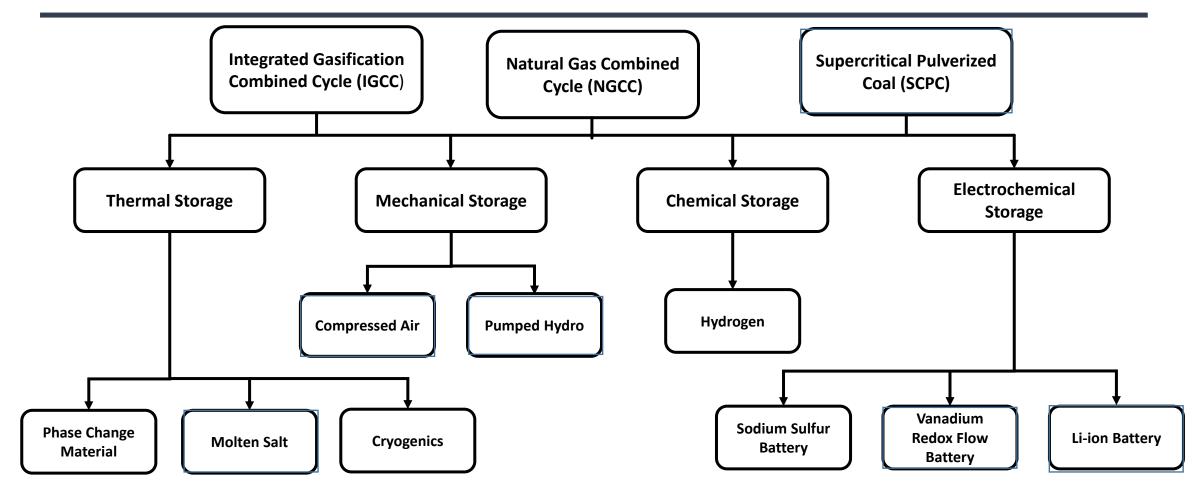


- Design Space
- Energy Storage Alternatives High Fidelity and Reduced Order Models
- Optimal Downselection
- Ongoing and Future Works



Design Space-Originally Proposed

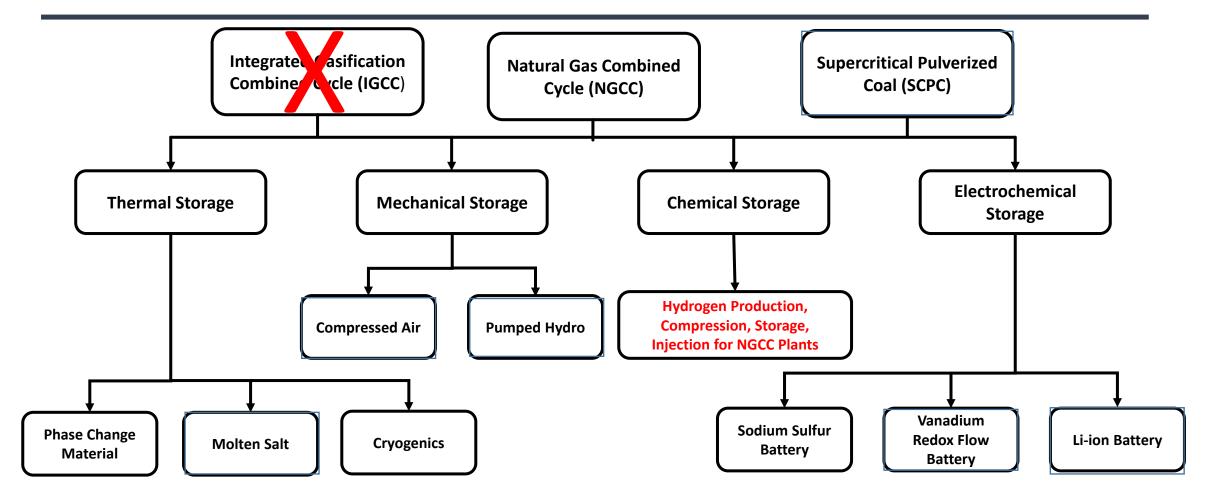






Design Space-Modified Proposed

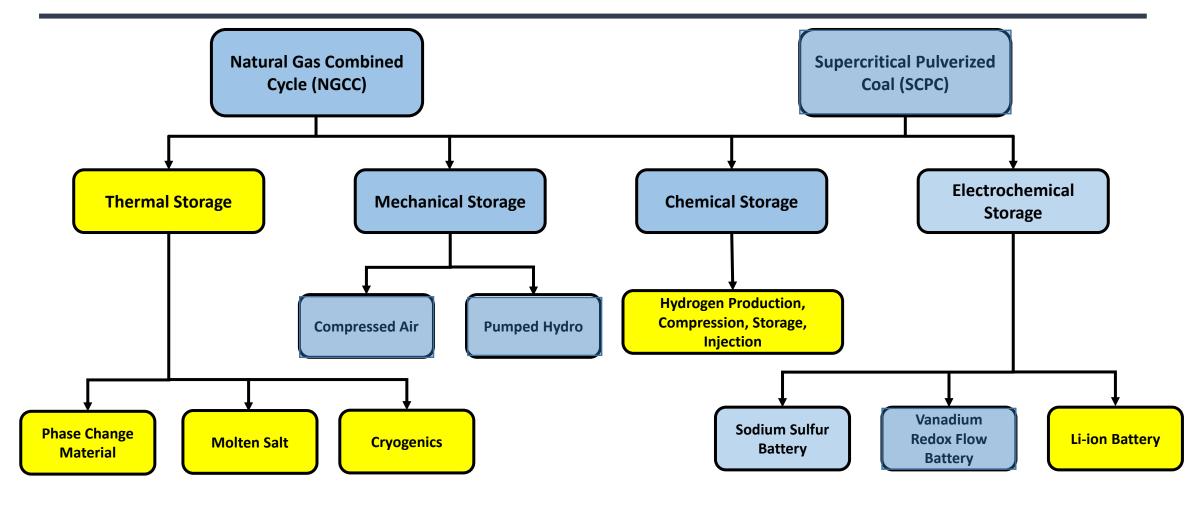






Design Space-Originally Proposed





Mostly Completed

Completed



Outline



- Design Space
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Reduced Order Models of NGCC and SCPC Power Plants





Reduced Order Modelling –NGCC Power Plant with H₂ Injection

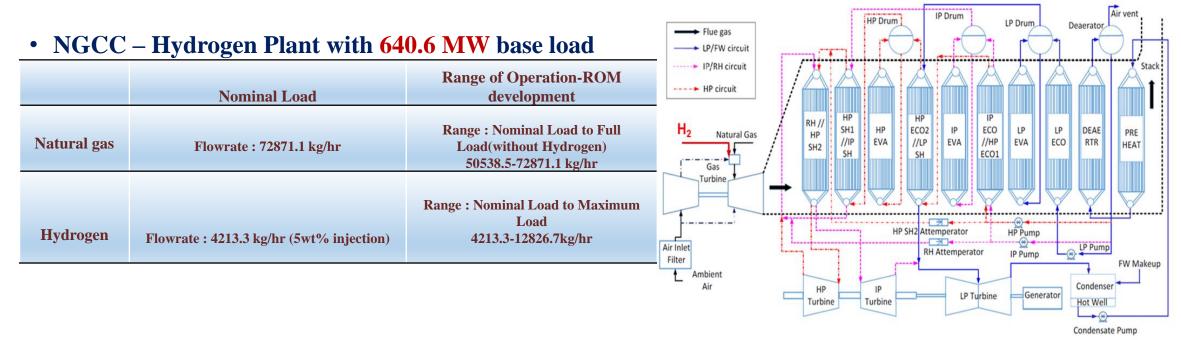


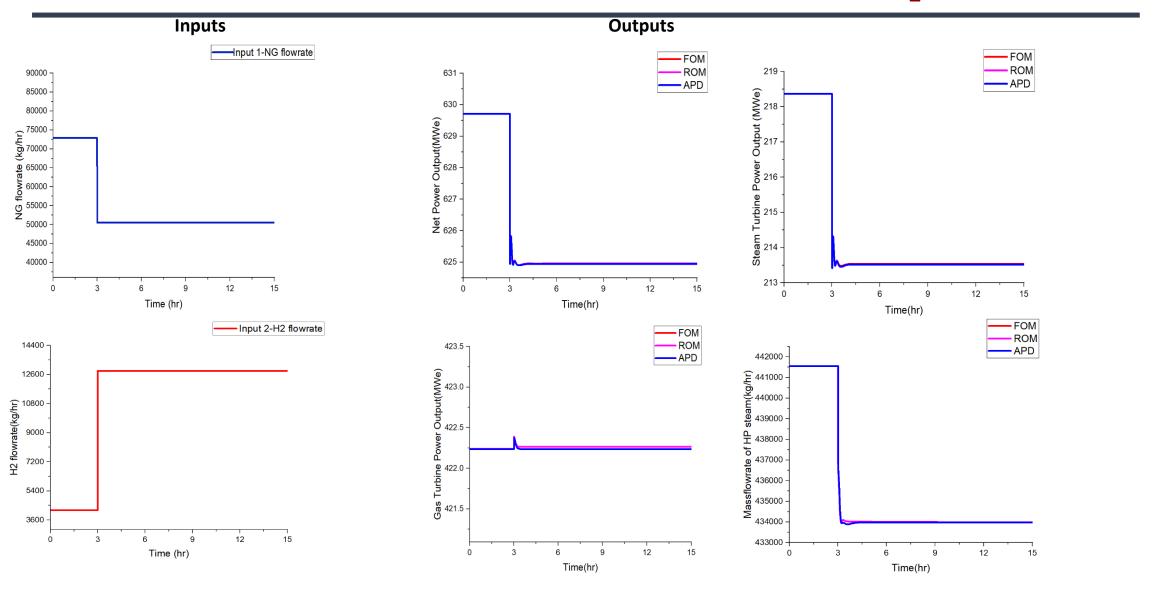
Fig 1. NGCC with Hydrogen Injection

- Discrete-time state space model developed by linearizing the nonlinear model
- Main Constraint: Hydrogen injection should be ≤ 20wt%





Model Validation- NGCC Power Plant with H₂ Injection





SCPC Plant Model-ROM development



SCPC Plant Key Variables

Parameter	Unit	SCPC Model	
Gross Power	MW	620	
Net Power	MW	532	
Main Steam Pressure	MPa	24.1	
Main Steam	°C	593	
Temperature	C		

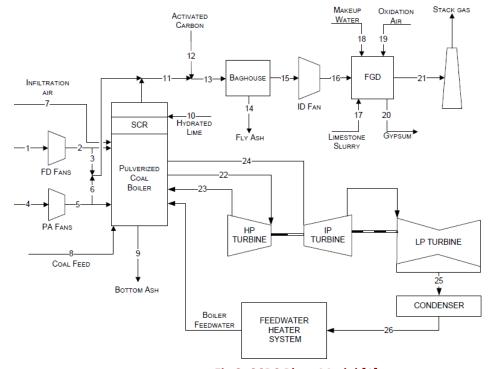


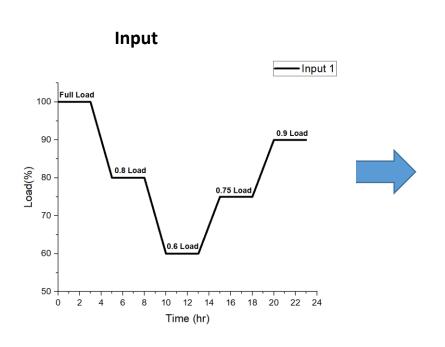
Fig 3. SCPC Plant Model [1]

- Highlights
- ✓ Reduced-order model generated using Hankel singular value (HSV) decomposition
- ✓ Range of operation for the ROM development evaluated between 60%-100% load.

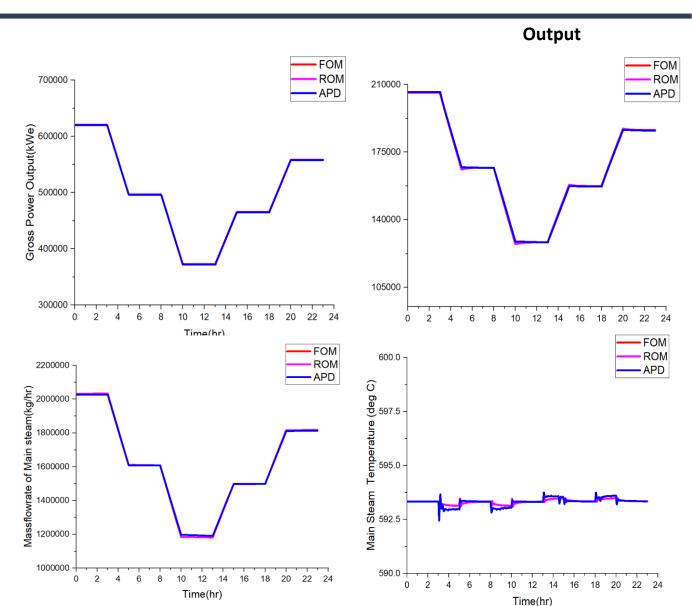


Reduced Order Modelling –SCPC Power Plant





APD: High-fidelity Aspen Plus Dynamic Model FOM: Full-order Model with 437 state variables ROM: Reduced-order Model with 14 state variables







Electrochemical Storage: Detailed and Reduced Order Models of High Temperature Sodium Sulfur Batteries



Sodium Sulfur Battery

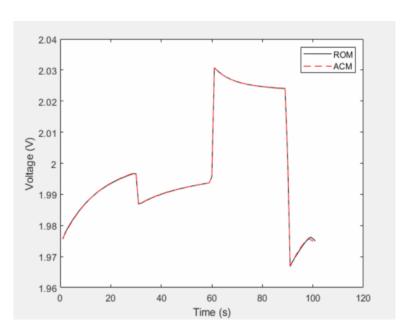


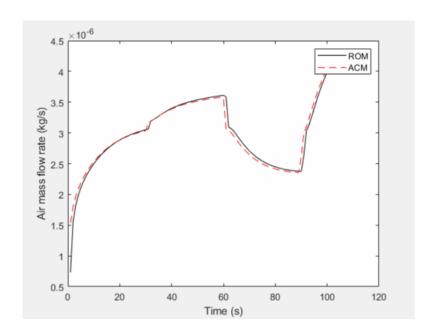
- Advantages:
 - High energy density (~150–240 Wh/kg) and power capacity (~90–230 Wh/kg)
 - High round-trip efficiency (~90%)
- Half cell reactions:

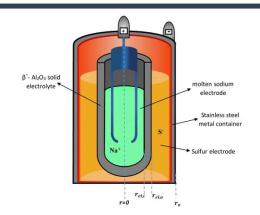
$$2Na \leftrightarrow 2Na^{+} + 2e^{-}$$

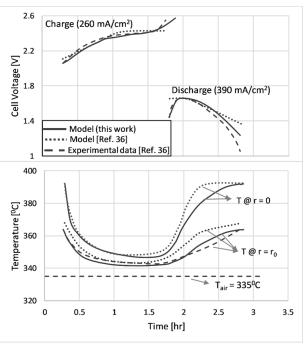
$$2Na^{+} + xS + 2e^{-} \leftrightarrow Na_{2}S_{x}$$

$$2Na + xS \leftrightarrow Na_{2}S_{x}$$









Schaefer (Caprio) S, Vudata S P, Bhattacharyya D, Turton R, "Transient Modeling and Simulation of a Nonisothermal Sodium-Sulfur Cell", 453, 227849, Journal of Power Sources, 2020





Electrochemical Storage: Detailed and Reduced Model of Vanadium Redox Flow Batteries







- VRFBs can offer practically unlimited energy storage
 - Nafion-115 ion exchange membrane
- Half-cell, overall reactions:

$$VO^{+2} + H_2O \leftrightarrow VO_2^+ + 2H^+ + e^-$$

 $V^{+3} + e^- \leftrightarrow V^{+2}$
 $VO^{+2} + H_2O + V^{+3} \leftrightarrow VO_2^+ + 2H^+ + V^{+2}$

- Vanadium cross-over reactions
 - Negative electrode

$$VO^{+2} + V^{+2} + 2H^{+} \rightarrow 2V^{+3} + H_2O$$

 $VO_2^{+} + 2V^{+2} + 4H^{+} \rightarrow 3V^{+3} + 2H_2O$

Positive electrode

$$V^{+2} + 2VO_2^{+} + 2H^{+} \rightarrow 3VO^{+2} + H_2O$$

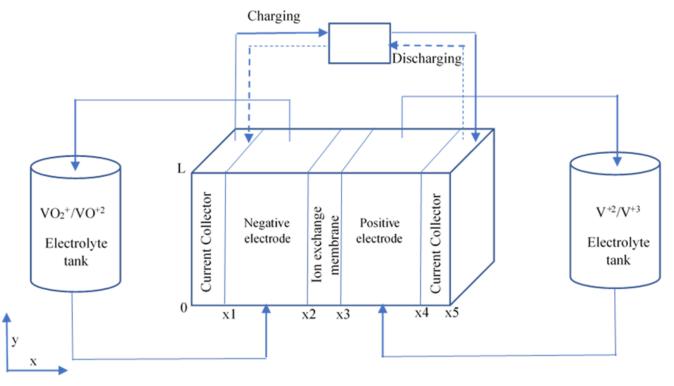
 $V^{+3} + VO_2^{+} \rightarrow 2VO^{+2}$

- Side reactions
 - Oxygen evolution at positive electrode

$$2H_2O \leftrightarrow O_2 + 4e^- + 4H^+$$

Hydrogen evolution at negative electrode

$$2H^+ + 2e^- \leftrightarrow H_2$$

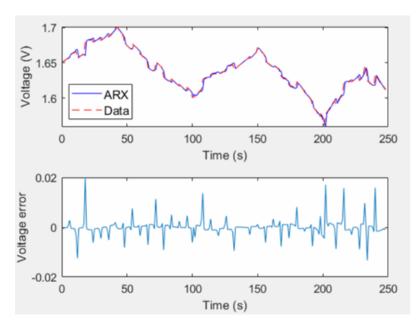


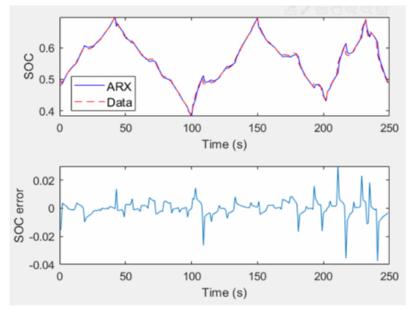


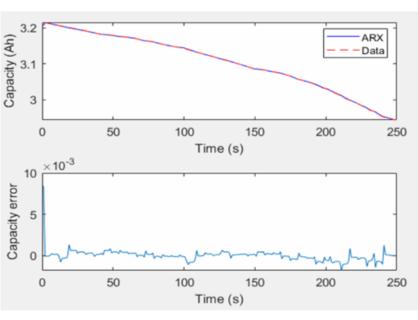
VRFB Surrogate Modeling



Reduced order model using a discrete-time state space model







Voltage Vs time

SOC Vs time

Capacity Vs time





Electrochemical Storage: Detailed Model of Li-Ion Battery





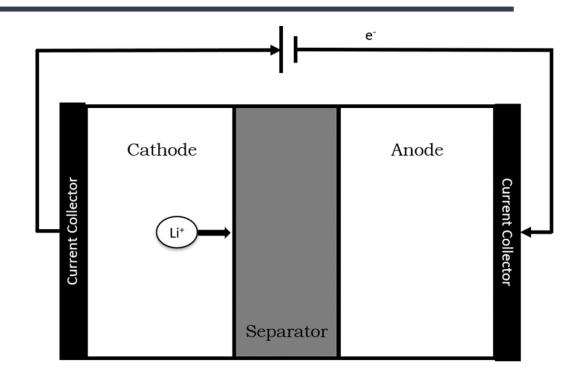


- Higher power, energy density, and longer cycle life compared to other electrochemical storages
- Positive electrode reaction:

$$LiMO_v \leftrightarrow MOy + Li^+ + e^-$$

Negative electrode reaction:

$$C_6 + Li^+ + e^- \leftrightarrow LiC_6$$



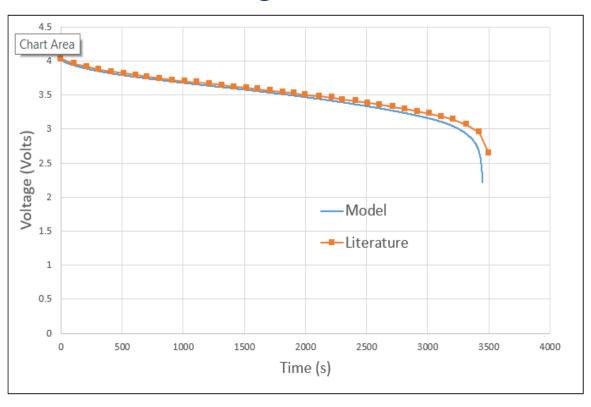
- Porous electrode pseudo two-dimensional model
 - Spatial and temporal variation of variables such as solid/liquid phase potentials and solid/liquid phase Li+ concentrations is modeled
 - Model based on concentrated solution theory
 - Solid phase reformulation using a parabolic approximation to reduce spatial dimensions
 - Coordinate transformation

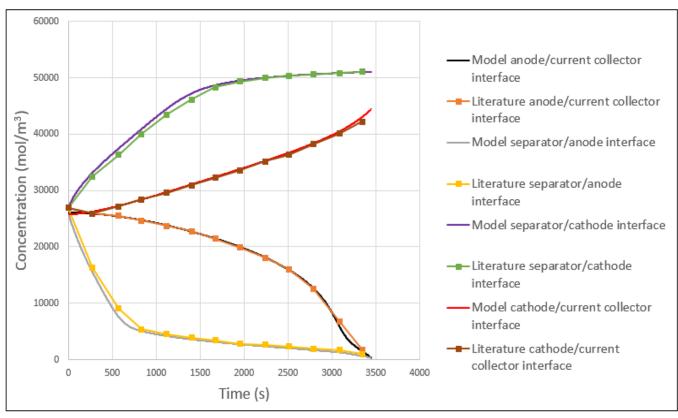




Model Validation – Li Ion Battery

- System of partial differential algebraic equations
- Simulated using Aspen Custom Modeler
- Validated using literature data*





Validation of Transients in Solid Phase Surface Concentration of Li lons under 1C Discharge

^{*} Northrop, P., Ramadesigan V., De S, Subramanian V., *Journal of the Electrochemical Society*, **158**, A1461-A1467 (2011).



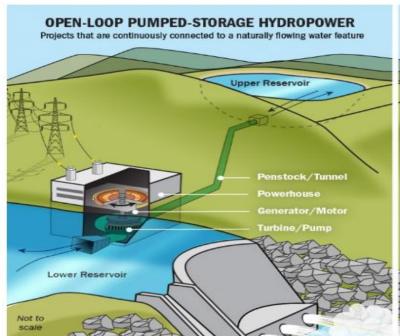


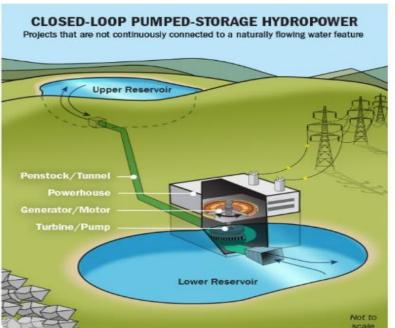
Mechanical Storage: Pumped Hydro

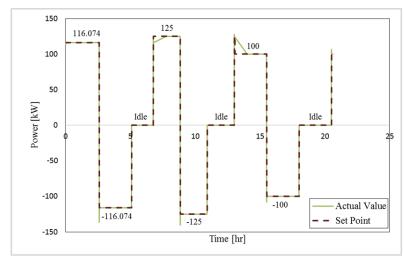


Types and Configurations









Load following power profile during generation and pumping modes with PID controllers

- two hydraulic machines
- two shafts
- two electric machines

Conventional PHS

- one hydraulic machine
- one shaft
- one electricmachine

Adjustable Speed PHS

- two hydraulic machines
- one shaft
- one electric machine

Ternary PHS https://www.energy.gov/ee re/water/pumped-storagehydropower



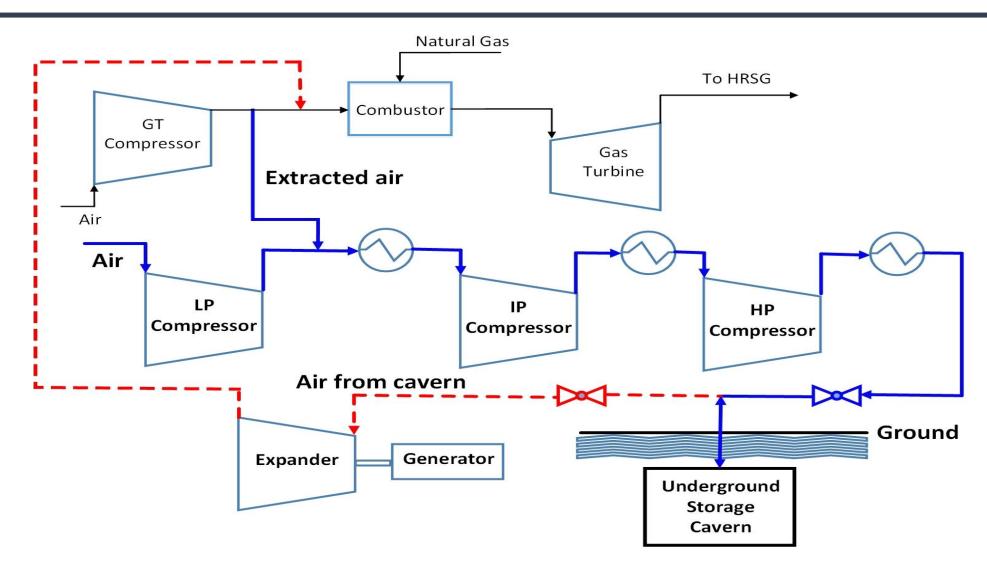


Mechanical Storage: Compressed Air Energy Storage



West Virginia University. Synergistic Mechanical Storage in an NGCC Plant **Using Compressed Air Energy Storage (CAES)**

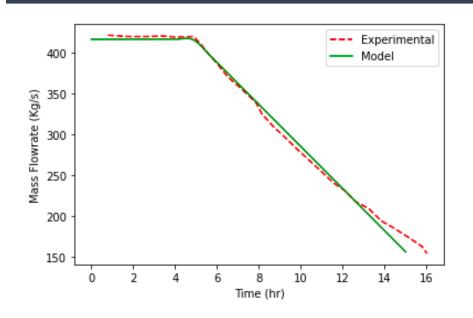


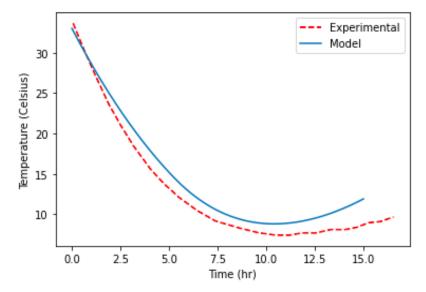




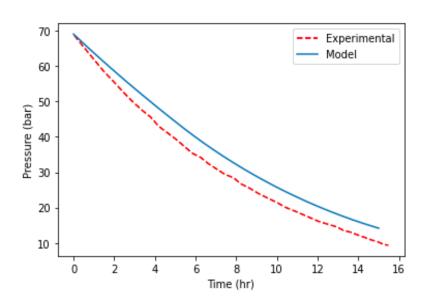








Discharge cycle of the Huntorf CAES simulated for 15 hr period



Experimental Data from: F. Crotogino, K.-U. Mohmeyer, and R. Scharf, "Huntorf CAES: More than 20 Years of Successful Operation," *Solut. Min. Res. Inst. Spring Meet.*, no. April, pp. 351–357, 2001.





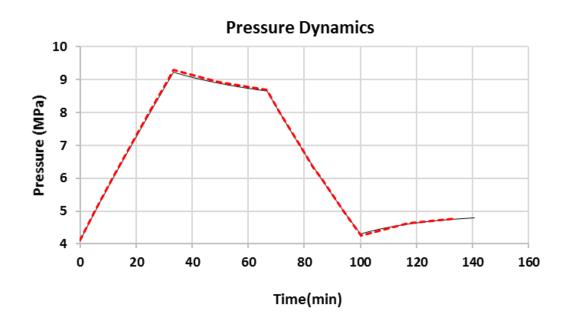
Chemical Storage: Hydrogen Storage

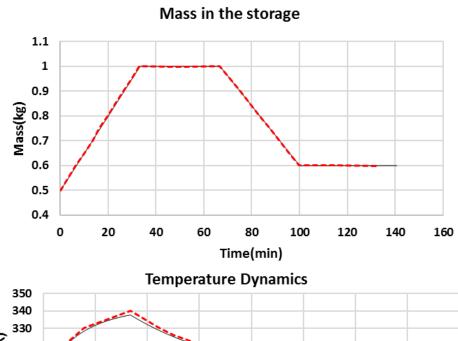


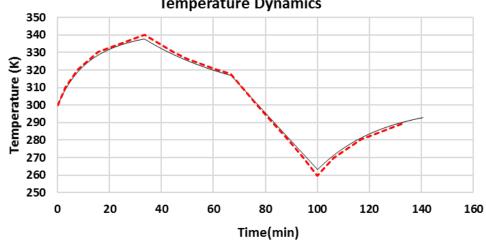


Hydrogen Storage Model- Validation with Literature Data

Constant Inflow and Outflow temperature ($T_{in} = T_{out} = T$) Charging and Discharging cycle (2 hr cycle)







Data from Literature: Xiao, J., Bénard, P., & Chahine, R. (2016). Charge-discharge cycle thermodynamics for compression hydrogen storage system. *International Journal of Hydrogen Energy*, 41(12), 5531–5539.





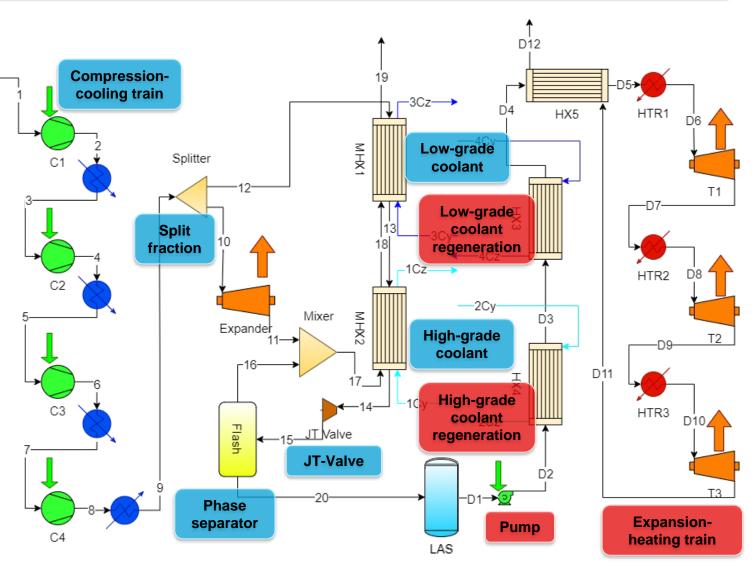
Cryogenic Energy Storage: Process Design, Simulation and Optimization



West Virginia University. Cryogenic Energy Storage: Heylandt Process **Flowsheet**



- **Charging cycle: liquefaction** & air storage
- **Inlet temperature to JT-valve** impacts the liquid air yield
- **Charging cycle: Coolant** regeneration
- **Expansion using air turbines** to generate work with intermediate heating
- Simulation and convergence challenges with several recycle loops

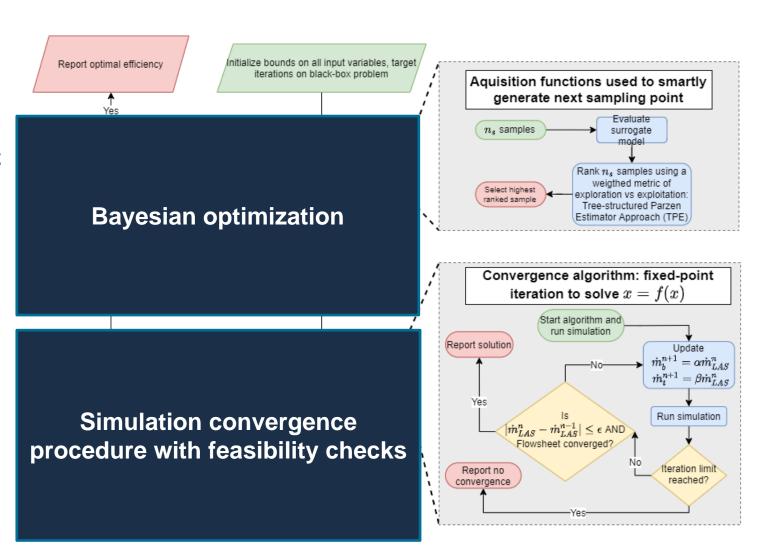






Simulation-based Optimization

- ASPEN Plus simulation for the CES cycle
- Bayesian optimization for exploration using acquisition functions to smart guess next sampling points
- Fixed point algorithm over pseudo input variables for simulation convergence at new sampling points
- Limited-memory Broyden– Fletcher–Goldfarb–Shanno algorithm (L-BFGS) for final refinement of local optima
- Automated in Python







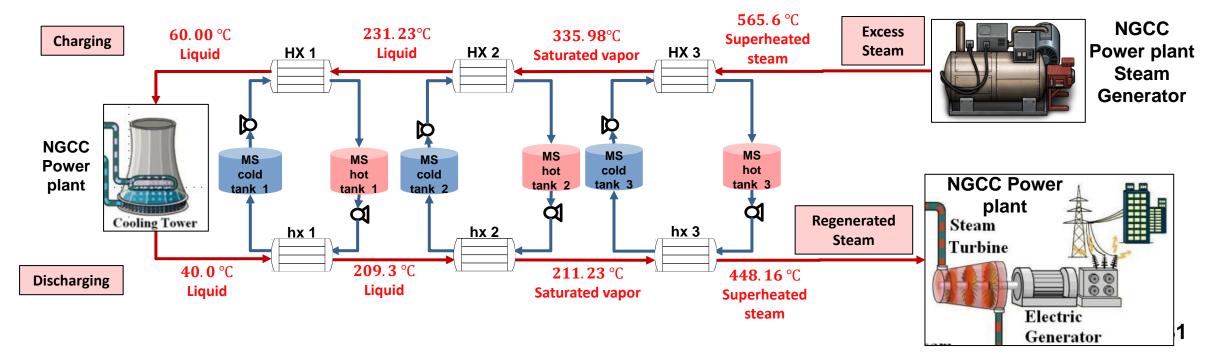
High Temperature Thermal Storage (Molten Salt-based Storage): Process Design, Simulation and Optimization





Steam Powered High Temperature Thermal Storage

- Energy is stored in the form of sensible/latent heat (e.g., molten salt, PCM)
- HTTS charges and delivers energy in the form of steam
- Storage medium circulates between cold and hot storage tanks
- More than one cycles are needed to achieve high round-trip efficiency
- Optimal synthesis of HTTS process cycle configurations
 - Process superstructure to embed all plausible process configurations
 - Mixed-integer nonlinear program (MINLP) to select optimal storage sizes and molten salts







Multiple Cycles Achieve High RTE

- The hot tank temperature needs to be high to be able to regenerate same quality (degree of superheat) of steam during discharging
- There is a trade-off between the salt temperature and storage efficiency suggested by one-cycle simulation

Molten salt flow rate	Hot tank temp.	Charging efficiency
Low	High	Low
High	Low	High

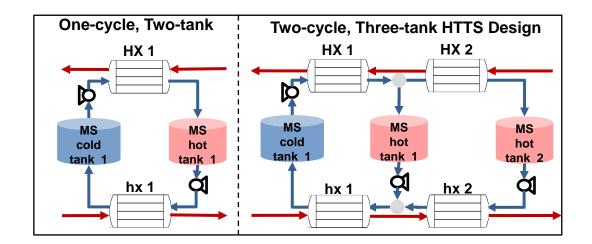
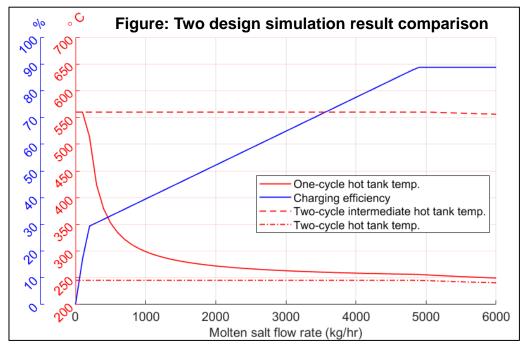


Table: Steam thermal properties in charging heat exchangers (41.15 bar, 565 °C)

40 bar steam	H1	H2	H3
Steam Energy Form	Liquid sensible heat	Latent heat	Vapor sensible heat
Steam Enthalpy KJ/kg	453	1713.5	793.7
Temperature Change	150- 250.4	250.4	250.4–565



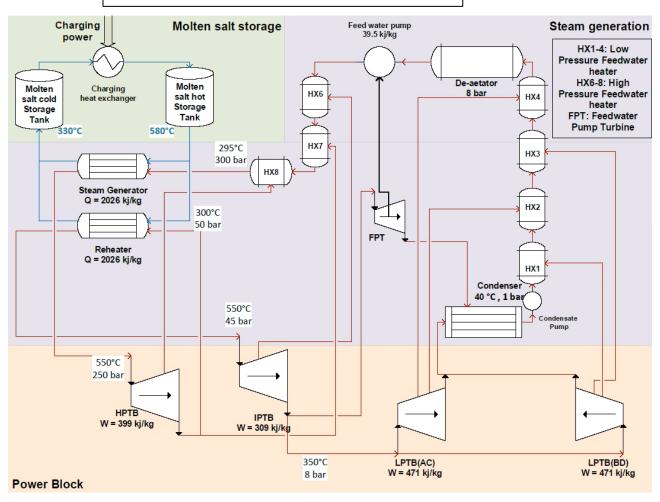




Electric Powered High-temperature Thermal Storage

- HTTS is charged by electrical heating
 - Molten salt is heated from 330°C to 580 °C
- Supercritical HTTS discharging converts energy from heat to electricity
 - Steam generation: Steam generator (boiler and superheater) and reheater are powered by hot molten salt
 - Power block: High, medium and lowpressure steam turbine
- Compared with steam powered HTTS
 - Pros: integration to power plant is less complicate and more adoptable
 - Cons: Lower efficiency and higher investment cost (additional power block)
- Comparing with Other Technologies
 - Lower LCOS but Lower efficiency
 - Requires more land space for discharging process
 - More cost-effective for large size storage

HTTS Round trip Efficiency:40.91%





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- Design Space
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- Optimal Downselection
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THESEUS: Technology Downselection Software Prototype

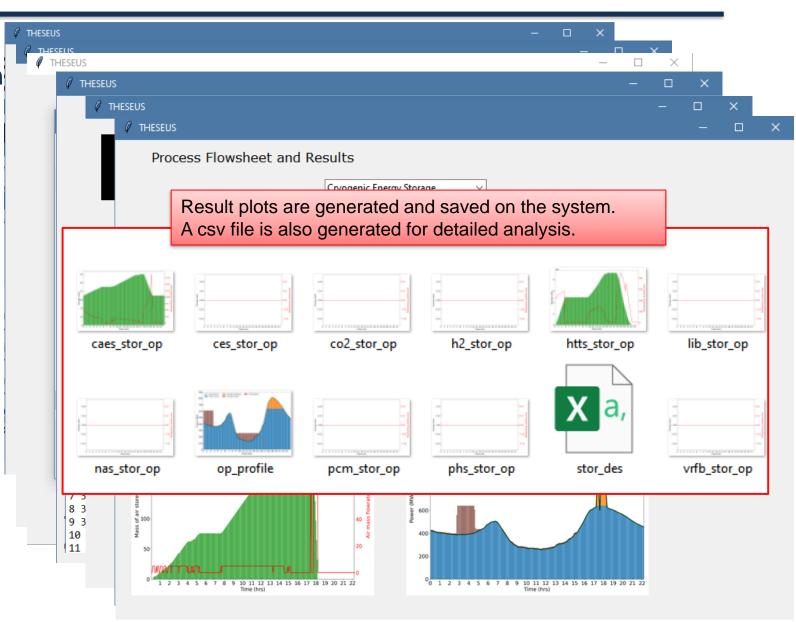
Inputs **THESEUS Framework Outputs Power plant model parameters Design of storage technologies** TecHno-Economic framework for Systematic Fixed and variable O&M costs Sizing of equipment in selected Energy Storage Utilization and downSelection energy storage technology Cycling costs for ramping Nominal capacity Minimum load factor **Power plant** -Storage states/flow decisions -Power and energy function model **Economic analysis** -Cost function parameters Levelized cost of storage for **Region specific parameters** selected technology Cost of electricity Based on inputs of power plant: Ambient conditions -Ramping costs Vanadium **CES** Redox Systems integration and optimization **Demand load profile** Individual technology optimal Li-ion H₂ - Discretized demand profile to **MINLP-based** configuration be met by the energy system **Downselection model** Sodium HTTS Sulfur Schedule for power plant Python interface Operational schedule for all **Pumped** systems to ensure demand GAMS back-end CAES Hydro profile is met Storage models 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23





THESEUS User Interface

- Application open page where user can select which technologies to integrate
- Update power plant model Inputs based on the power plant design for integration
- Upload Demand profile as csv
- Solve Downselection model in GAMS using the selected technologies for integration
- Results are obtained on the Analysis page
- For detailed analysis, user can visit the Results folder







Framework Back-End: Optimization Formulation

$$\min TC = \sum_{i=1}^{NI} \left(C_i^{S,iv} + C_i^{S,of} + \sum_{t=1}^{NT} \left(C_{i,t}^{S,ov} + C_{i,t}^{FP,ov} \right) + C_t^{FP,rc} + C^{os} + C^{us} \right)$$

Objective: Minimizing total system cost

Grid-level constraints



Energy balance

Electricity oversupply/undersupply penalty

Power plant model



General operational model

General cost model

Ramping constraints

Efficiency model

Capacity constraints

Operating and fuel cost

Ramping cost





Technology-specific models

General operational model

Constraints on power output

Energy balance

Power model

Energy model

Operational mode

Constraints on energy output

Cyclical constraint on energy stored

0700

General cost model

Investment cost

Fixed cost

Variable cost





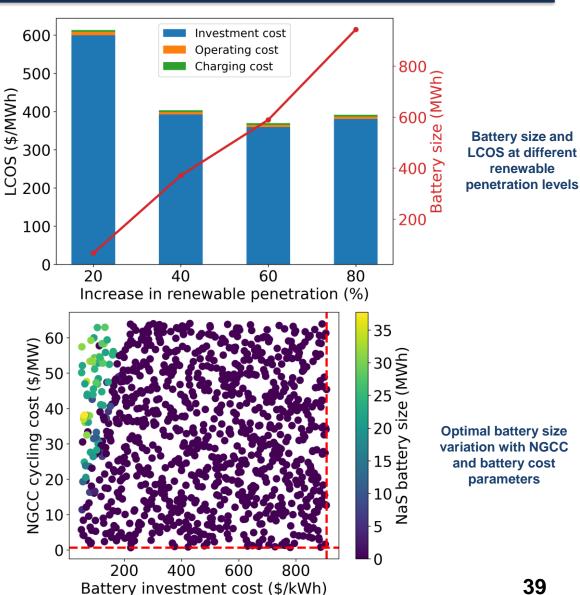
Sodium Sulfur Battery Integration Results

- Integration not optimal for "normal day" due to high investment cost
- 80% increase in renewable penetration to justify investment in large-scale storage
- Based on cost sensitivity analysis, for battery selection:

NGCC specific cycling cost (\$/MW) Unit battery investment cost (\$/kWh)

LCOS: \$391/MWh

Efficiency: 85%





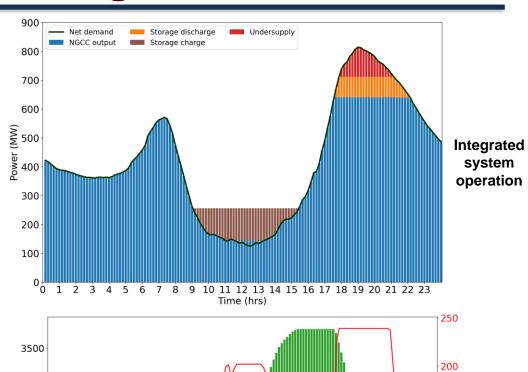


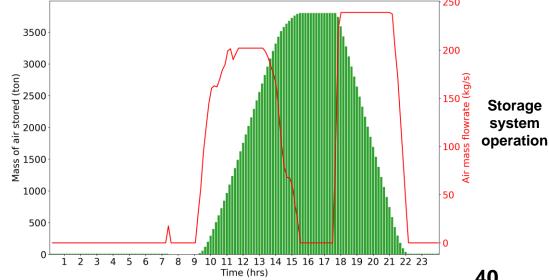
Cryogenic Energy Storage Integration Results

- Integration optimal to enable peakshaving for 80% increase in demand variability
- Optimal storage design capacity: 71 MW/283 MWh
- Unmet demand due to upper bound on storage size
- Future analysis: Multiple CES storage systems to meet demand spike

LCOS: \$201/MWh

Efficiency: 52%







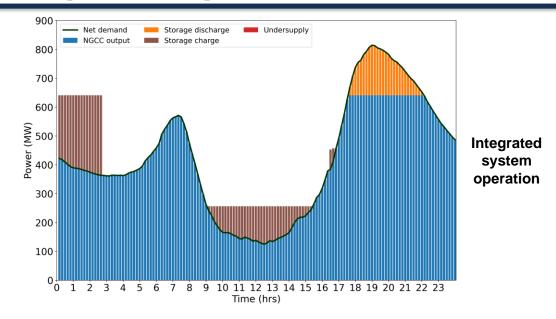


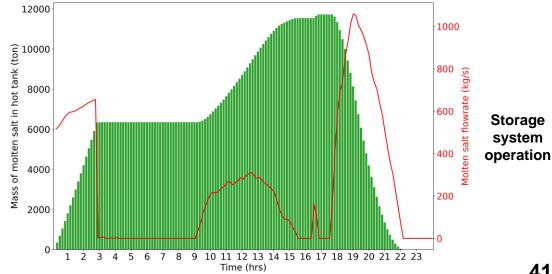
Molten Salt Thermal Storage Integration Results

- Integration optimal to enable peakshaving for 80% increase in demand variability
- Optimal storage design capacity: 173 MW/483 MWh
- **Demand peak above NGCC nominal** capacity completely met by power discharged by storage
- Technology suitable for low-cost largescale storage

LCOS: \$135/MWh

Efficiency: 39%









Compressed Air Energy Storage Integration Results

Compressor inlet/turbine outlet

pressure: 30 bar, Cavern operating

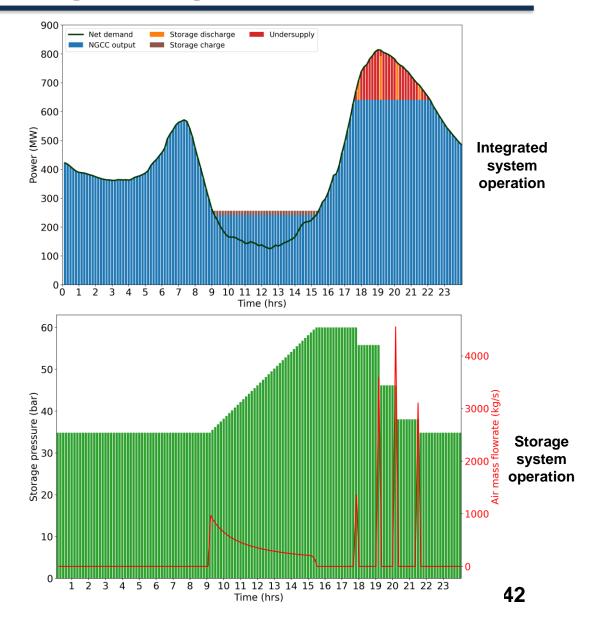
pressure: 30-60 bar

– Max pressure ratio: 2

- Pressure increases from 30 to 60 bar with small amount of charging: reduced storage capacity
- Although high round-trip efficiency (65%), max pressure ratio of 2 restricts the energy output and increases costs

LCOS: \$216/MWh

Efficiency: 67%







Results Summary

Among the technologies considered so far, following is the rank order of storage technologies as per the cost (LCOS):

No.	Technology	Round-trip efficiency (%)	LCOS (\$/MWh)
1	Molten salt thermal storage	39	135
2	Cryogenic energy storage	52	201
3	Compressed air energy storage	67	216
4	Sodium sulfur battery	85	391

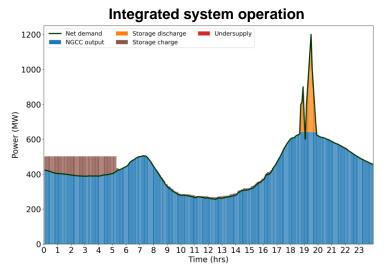
This trend is inverse to what we may expect from the storage efficiency!

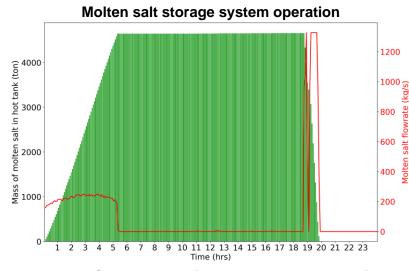


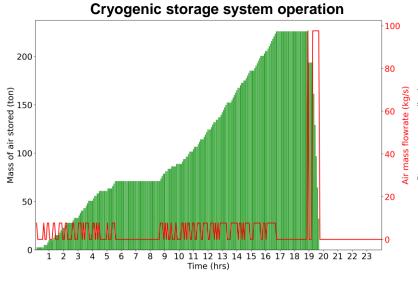


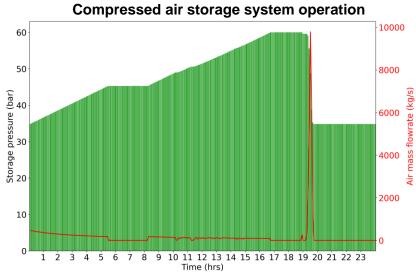
Downselection: Case Study 1

- Demand profile with extreme spike higher than NGCC nominal capacity
- Top 3 technologies considered for integration : CES, HTTS, CAES
- All 3 technologies selected
- Storage sizes and LCOS:
 - CES: 29 MW, \$493/MWh
 - HTTS: 217 MW, \$203/MWh
 - CAES: 313 MW, \$374/MWh
- CAES has highest LCOS for stand-alone integration, but cheaper than CES in downselection











Ongoing and Future Works



- Complete remaining ROM development
- Complete downselection
- Complete detailed dynamic simulation of promising storage technologies
- Complete detailed techno-economic analysis of promising storage technologies



Acknowledgement



- Gratefully acknowledge funding from DOE-NETL through Grant#DE-FE0031771 tited "Techno-Economic Optimization of Advanced Energy Plants with Integrated Thermal, Mechanical, and Electro-Chemical Storage"
- Support from NETL project manager Matthew Adams
- Our students: Manali Zantye (TAMU), Mengdi Li (TAMU), Akhilesh Gandhi (TAMU), Yifan Wang (WVU) and Sai Pushpitha Vudata (WVU), Alex Gentile (WVU), Pavitra Senthamilselvan Sengalani (WVU)





Thank you for your attention

Questions?