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High-Fidelity and High-Performance Computational Simulations for Rapid Design Optimization of Sulfur Thermal Energy Storage

Program: HPC4EI (High Performance Computing for Energy Innovation)

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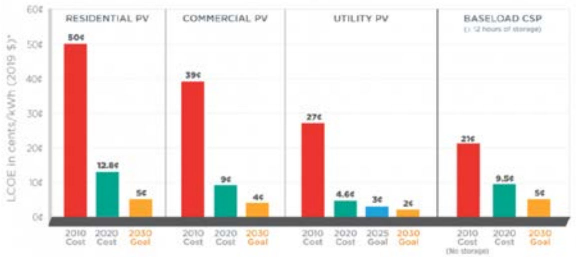
Sulfur based energy storage

Current methods of storage

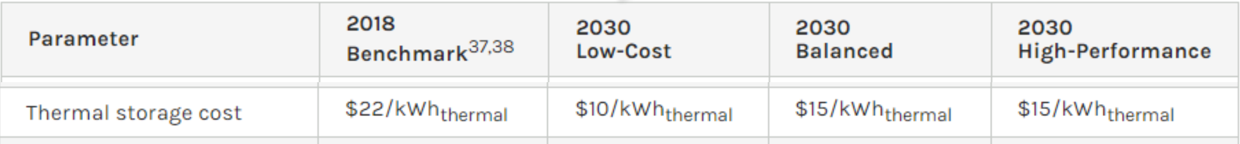
- Two-tank solar salt storage concept for the IPH temperature range of 100-300 °C is prohibitively expensive
- Latent-based phase change materials (PCMs) and sensible-based solid-state thermal storage media (concrete, rocks) suffers **from high storage cost, poor thermal responsiveness, and/or thermal cyclic stability concerns.**


Solar Energy Technologies Office Progress and Goals
Photovoltaics (PV) and Concentrating Solar-Thermal Power (CSP)

*Levelized cost of energy (LCOE) PV progress and targets are calculated based on average U.S. climate and without the investment Tax Credit or state/local incentives.

Table IV. Benchmark parameters for a 100 MW CSP system with 14 hours thermal storage.[36]

Parameter	2018 Benchmark[37,38]	2030 Low-Cost	2030 Balanced	2030 High-Performance
Net power-cycle efficiency	37%	40%	50%	55%
Rated thermal power	730 $\text{MW}_{\text{thermal}}$	675 $\text{MW}_{\text{thermal}}$	540 $\text{MW}_{\text{thermal}}$	491 $\text{MW}_{\text{thermal}}$
Power block cost	$\$1330/\text{kW}_{\text{ac-gross}}$	$\$700/\text{kW}_{\text{ac-gross}}$	$\$900/\text{kW}_{\text{ac-gross}}$	$\$900/\text{kW}_{\text{ac-gross}}$
Solar field cost	$\$140/\text{m}^2$	$\$50/\text{m}^2$	$\$50/\text{m}^2$	$\$70/\text{m}^2$
Site preparation cost	$\$16/\text{m}^2$	$\$10/\text{m}^2$	$\$10/\text{m}^2$	$\$10/\text{m}^2$
Tower and receiver cost	$\$137/\text{kW}_{\text{thermal}}$	$\$100/\text{kW}_{\text{thermal}}$	$\$120/\text{kW}_{\text{thermal}}$	$\$120/\text{kW}_{\text{thermal}}$
Thermal storage cost	$\$22/\text{kWh}_{\text{thermal}}$	$\$10/\text{kWh}_{\text{thermal}}$	$\$15/\text{kWh}_{\text{thermal}}$	$\$15/\text{kWh}_{\text{thermal}}$
Levelized O&M cost[39]	$\$9/\text{kW}_{\text{thermal}}\text{-yr}$	[illegible]8/$\text{kW}_{\text{thermal}}\text{-yr}$	$\$7/\text{kW}_{\text{thermal}}\text{-yr}$	$\$7/\text{kW}_{\text{thermal}}\text{-yr}$
Levelized capacity factor	68.9%	69.2%	70.7%	71.0%
LCOE (2019 US$)[40]	**[illegible].8¢/kWh**	**5.0¢/kWh**	**5.0¢/kWh**	**5.0¢/kWh**



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Sulfur based storage*

- Sulfur is a cheap commodity at $80/ton compared to $1100 - 1300/ton for conventional salts and costs around 2-3 $/kWh
- High energy storage density
- Sulfur-based TES have 3-14 times higher charge-discharge rates than PCM-TES

✓ Less than DOE target of $\$15/\text{kW}_{\text{th}}$ for thermal storage^{+}

✓ Better performance

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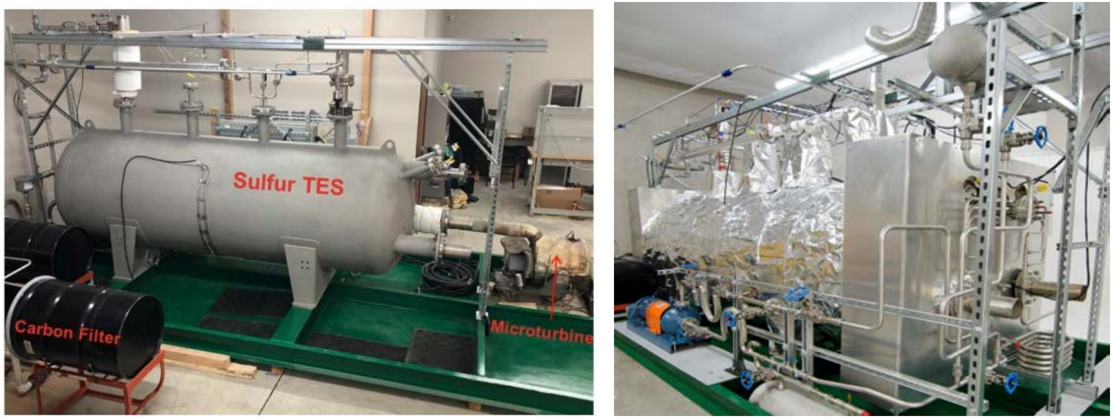
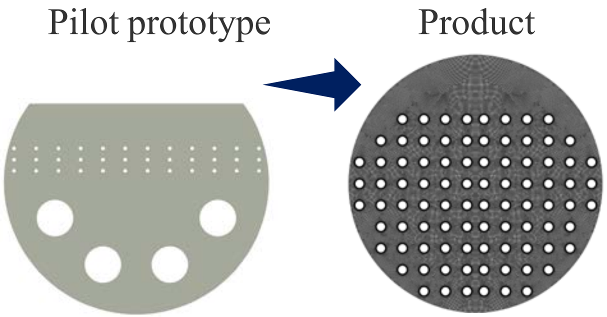
* Nithyanandam, Karthik, et al. No. DE-FE0032007-Element16-Final Report. Element 16 Technologies, Inc., Glendale, CA (United States), 2022.
+ Murphy, Caitlin, et al. National Renewable Energy Lab.(NREL), Golden, CO (United States), 2019.

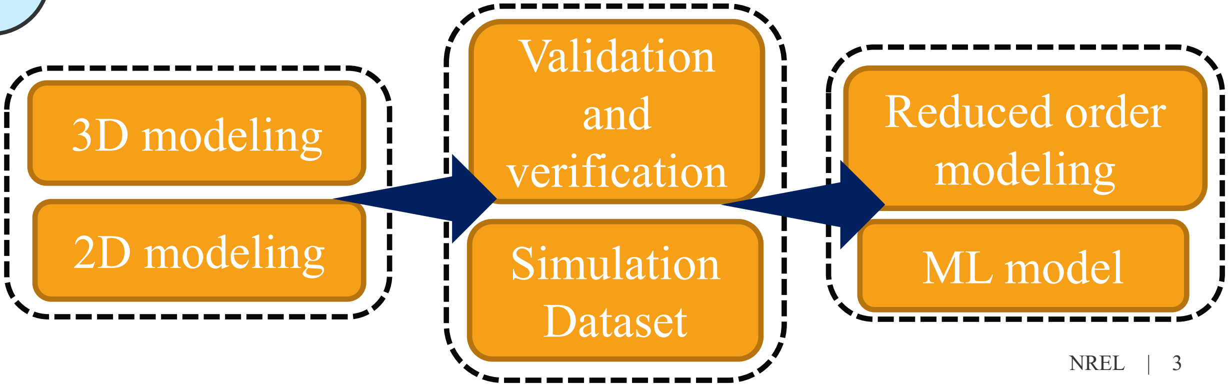
Sulfur TES Study design

- **Goals:**
    - Validate Numerical model
    - Design either correlation for HTC/Temperature behavior of sulfur with time (charge/discharge)
    - Develop tool to predict design of TES for a given thermal output of the system (product aimed at IPH application)



Element 16's 350KWh pilot sulfur TES prototype





3D modeling

2D modeling

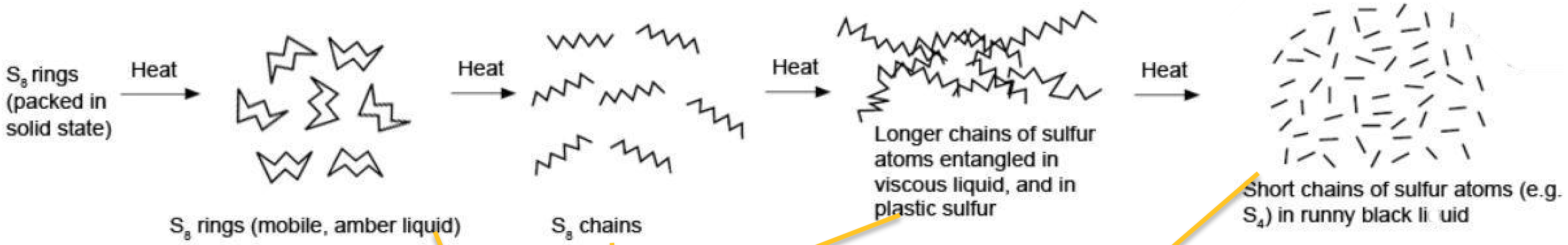
Validation and verification

Simulation Dataset

Reduced order modeling

ML model

Sulfur properties



S_8 rings (packed in solid state)

Heat

S_8 rings (mobile, amber liquid)

Heat

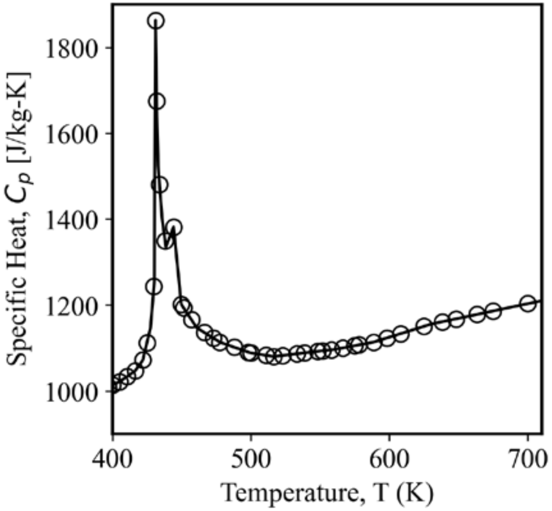
S_8 chains

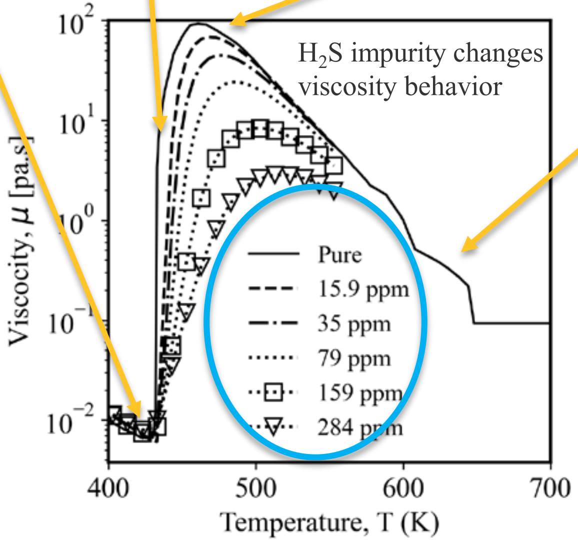
Heat

Longer chains of sulfur atoms entangled in viscous liquid, and in plastic sulfur

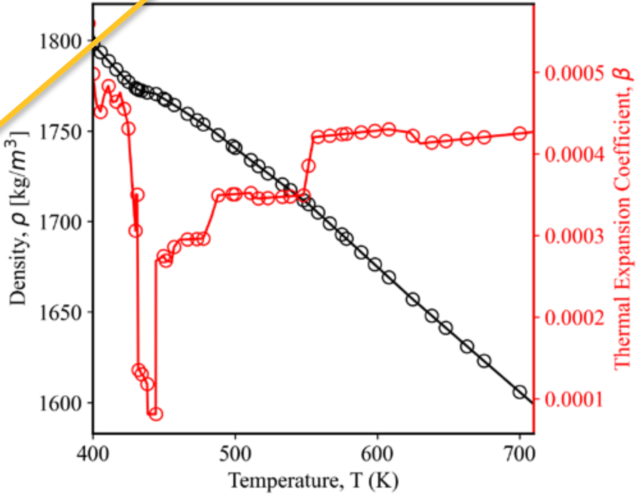
Heat

Short chains of sulfur atoms (e.g. S_4) in runny black liquid

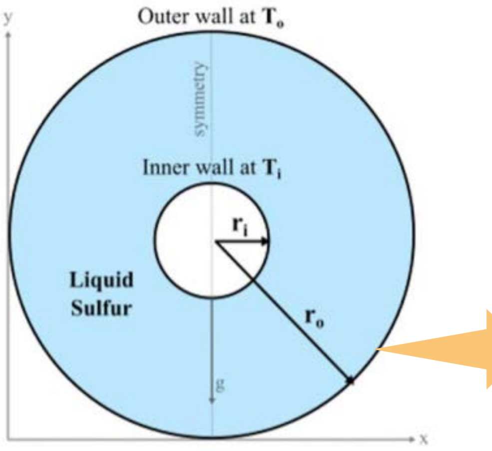


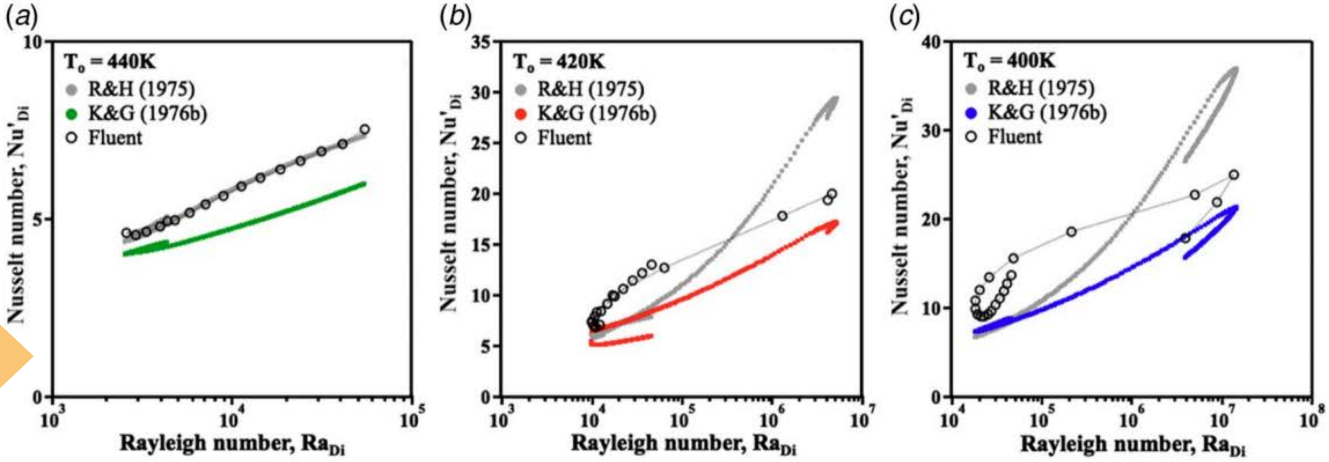


H_2S impurity changes viscosity behavior



Why not empirical correlations?





Correlation failure for commonly known two-cylinder Nu-Ra correlations because of,

- Heat transfer ability of sulfur begins to show unconventional fluctuations with respect to temperature gradient as sulfur chains break apart.
- Rapid shifts in sulfur viscosity with increasing temperature
- Heat transfer physics and convective flow behaviors of the fluid are significantly altered with change in viscosity
- Resulting in an unpredictable and highly nonuniform distribution of fluid properties throughout the TES.

Oliver, Madeleine C., et al. *Journal of Energy Resources Technology* 145.12 (2023): 121704.

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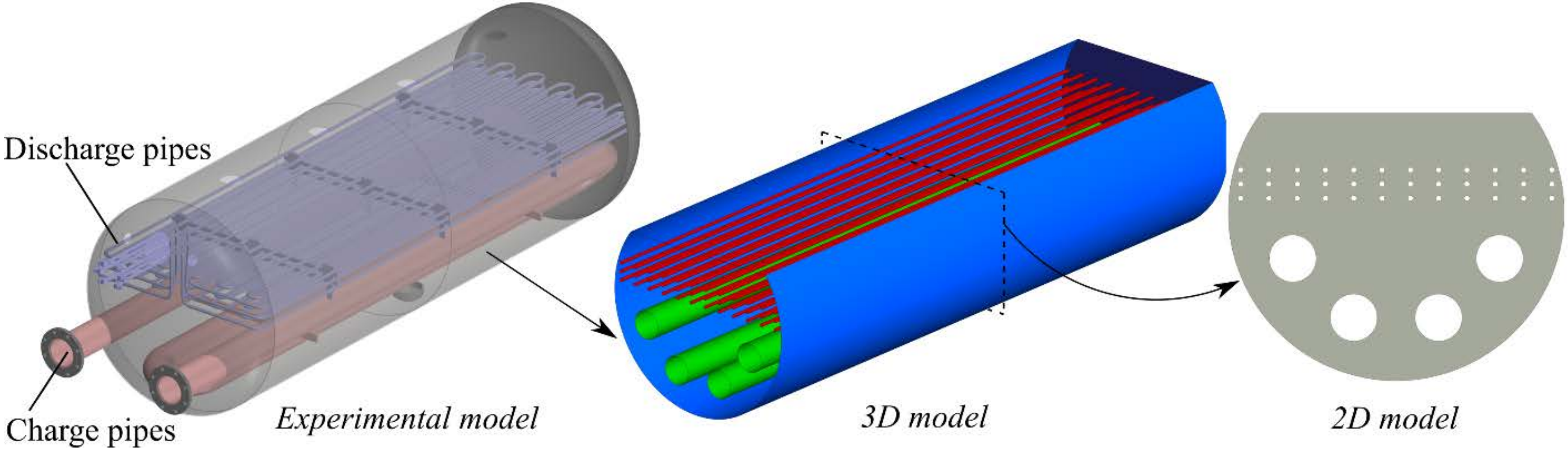
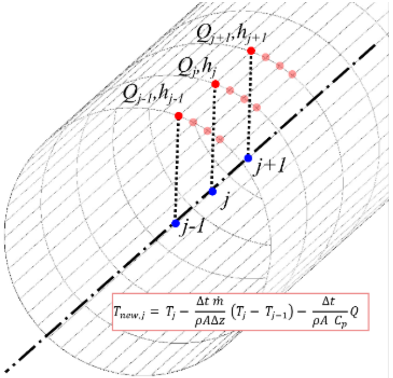
Modeling approach





$$T_{new,j} = T_j - \frac{\Delta t\, \dot{m}}{\rho A \Delta z}\left(T_j - T_{j-1}\right) - \frac{\Delta t}{\rho A\ C_p} Q$$

HTF temperature profile predicted by UDF

Heat transfer rate at the wall of tube *j*

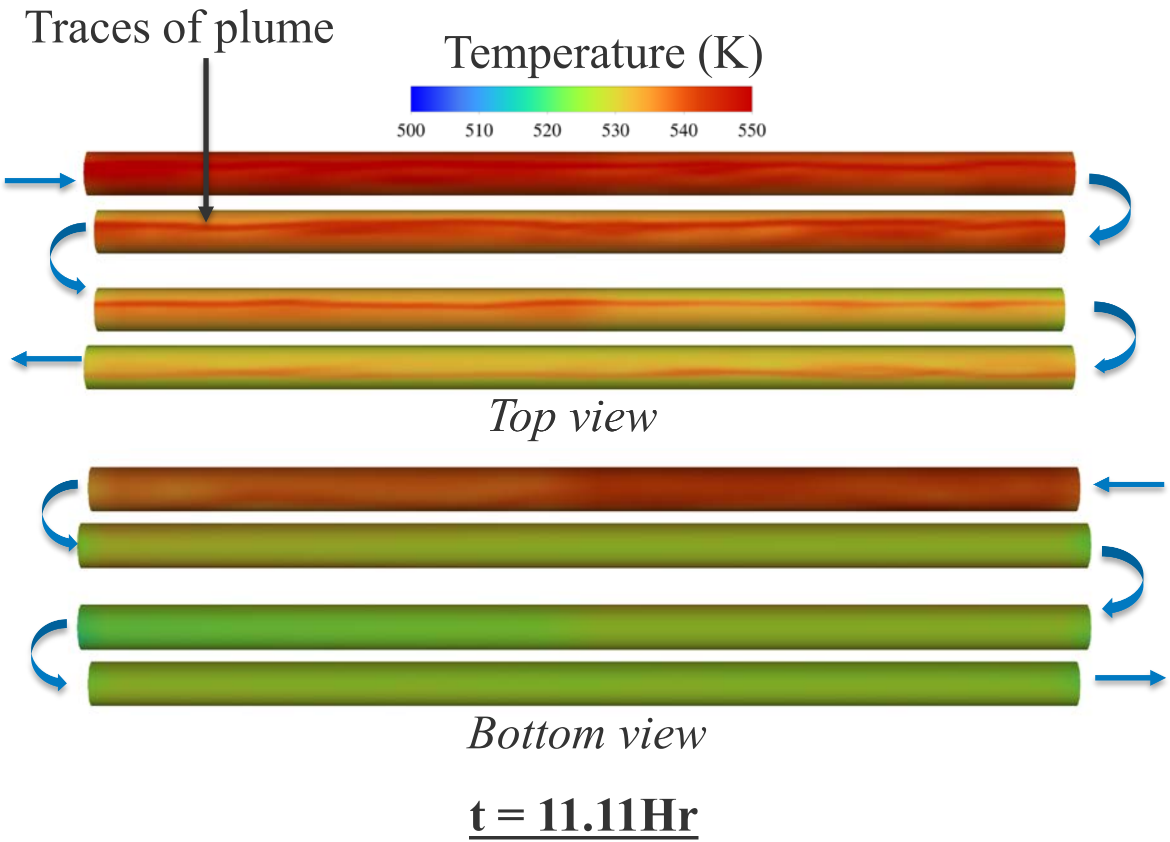
$$\rho C_p A_c \frac{\boxed{\partial T_f(z,t)}}{\partial t} + \dot{m} C_p \frac{\partial T_f(z,t)}{\partial z} = \boxed{-Q_{tube,j}(z,t)}$$

Explicit finite difference methods

Sum of heat transfer rates for all tube wall mesh elements in the CFD model assigned to reduced-order model axial element *i*

$$T_f^{i,t+1} = T_f^{i,t} - \frac{\dot{m}\Delta t}{\rho A_c \Delta z}\left(T_f^{i,t} - T_f^{i-1,t}\right) - \frac{\boxed{Q_{tube}^{i,t}}\Delta t}{\rho C_p A_c}$$

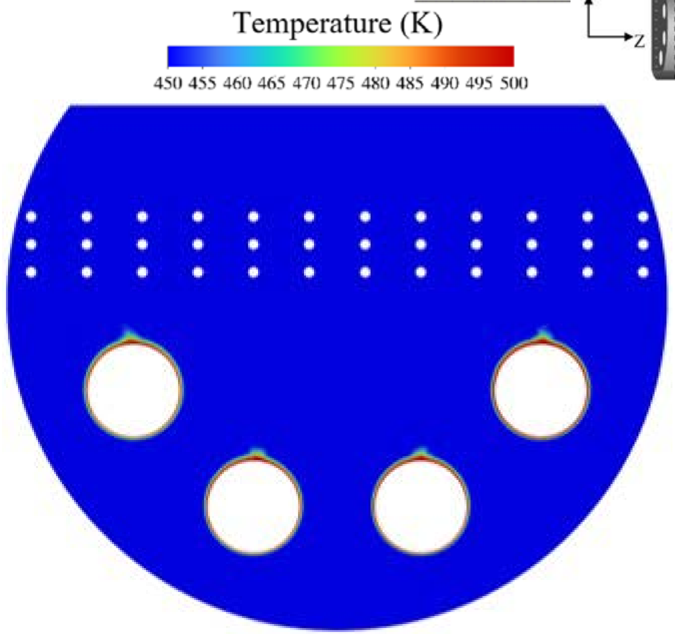
Temperature profile

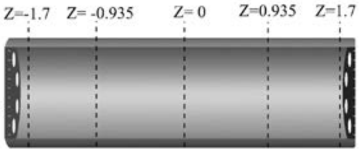


Temperature gradient across charge pipes based on the convective boundary condition.

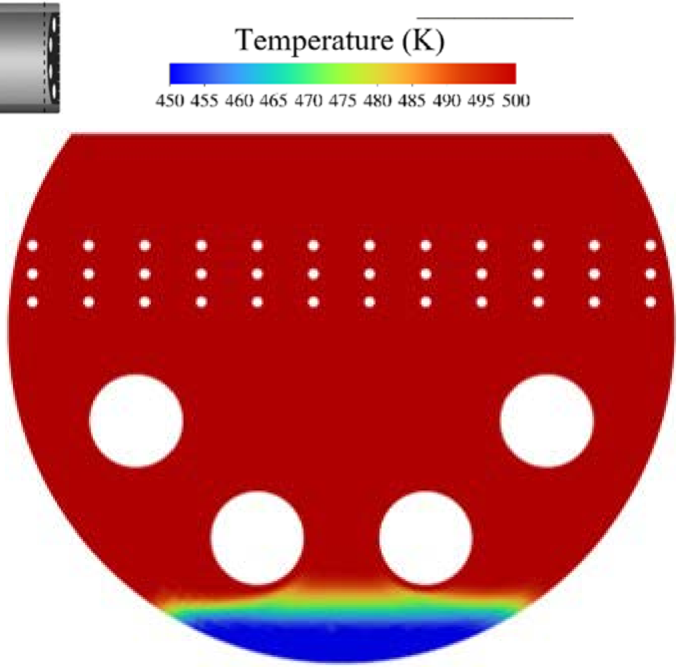
- Air at higher temperature enters charge pipes, navigates through four passes, and exits with lower temperature by charging sulfur inside domain to higher temperature.
- Top view of the charge pipes demonstrates traces of high temperature location across the length, elucidating convection of sulfur and location of plume detachment from charge pipe.
- Evident temperature difference in top and bottom view of charge pipes facilitates natural convection occurring through radial temperature gradient.

3D simulations - Charge and Discharge



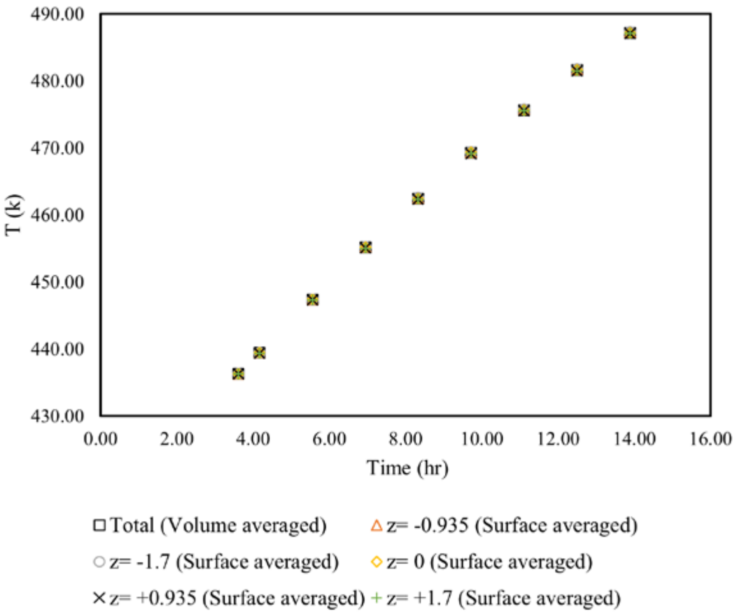


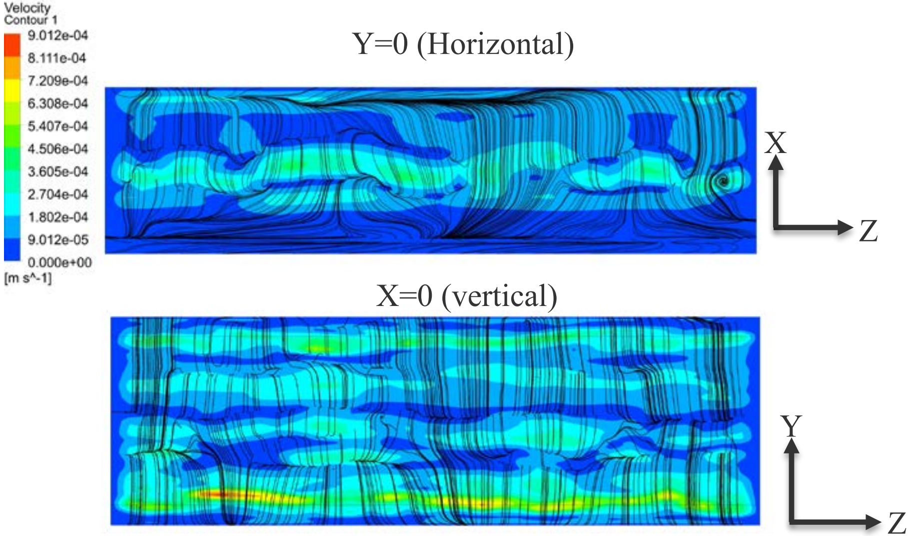
t = 3.6 to 13.8 hr at
Midplane(z=0) of tank



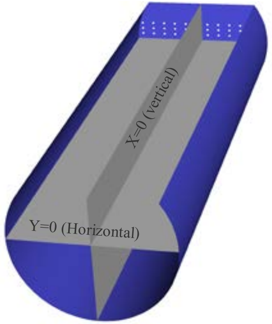
t = 20.8 to 26.8 hr at
Midplane (z=0) of tank

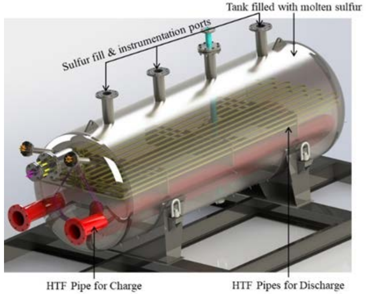
3D simulations- Axial and cross flow





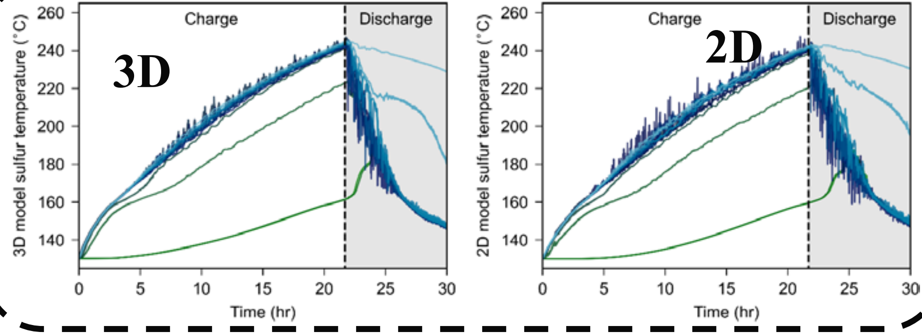
- 2D cross section from the prototype tank can give an accurate representation of the bulk average temperature and viscosity in tank
- The two-dimensionality of heat transfer mechanism within the TES can be useful in ML modeling and optimization of system





Summary of Modeling

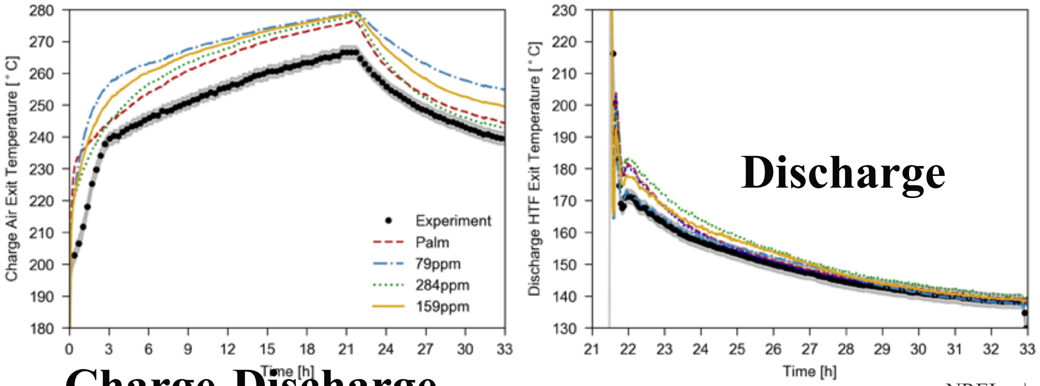
3D vs 2D



- Computations capture physical TES behavior
- Outlet temperature measurement had heat loss

- Absence of three dimensionality in sulfur TES
- 2D simulation can be used for ROM and optimization.

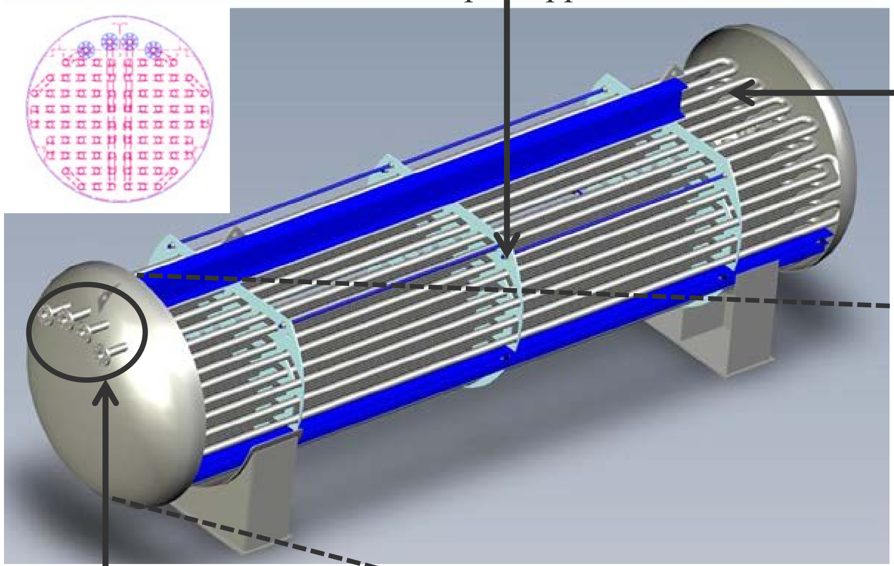
Computation vs Exp



Discharge

Charge-Discharge

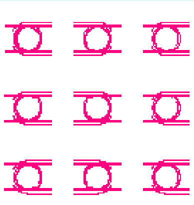
Sulfur TES Design for solar thermal integration



Baffles for Pipe Support

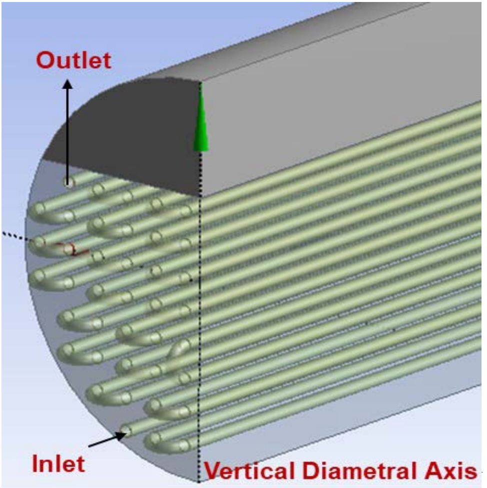
HTF (thermal oil) Pipe Circuit

Interface to HTF Pipe Circuits



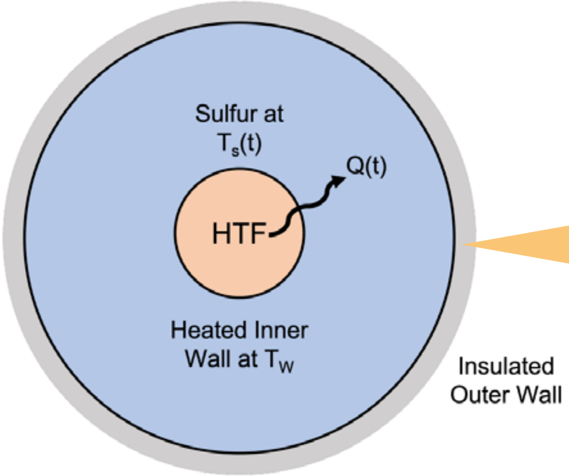
Model unit-cell confirmation to predict the total TES performance??

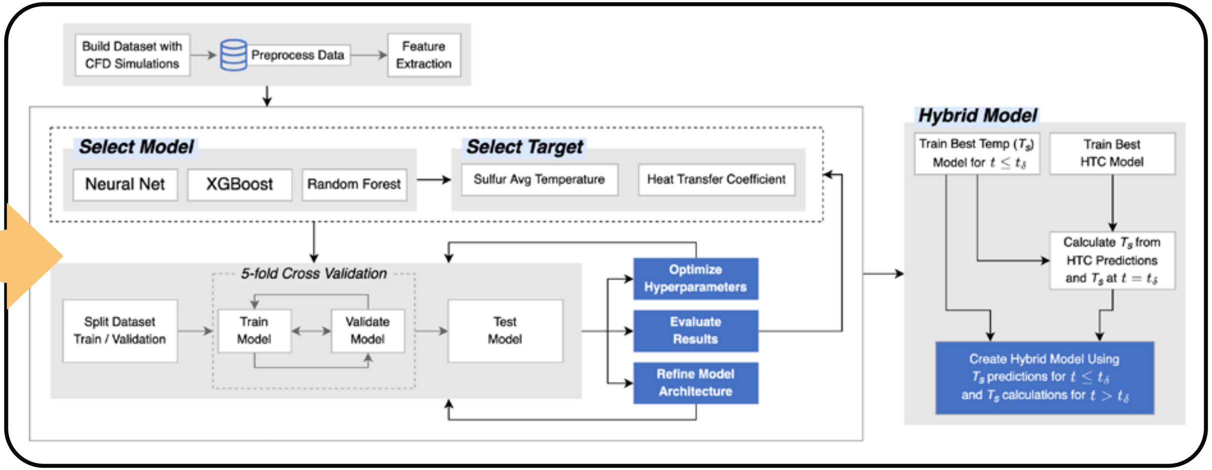
During discharge cold HTF enters from the bottom and exits from the top. During charge, the flow direction is reversed



Schematic depicted here for a 1.5 MWh system that is being built

Surrogate Model





Build Dataset with CFD Simulations → Preprocess Data → Feature Extraction

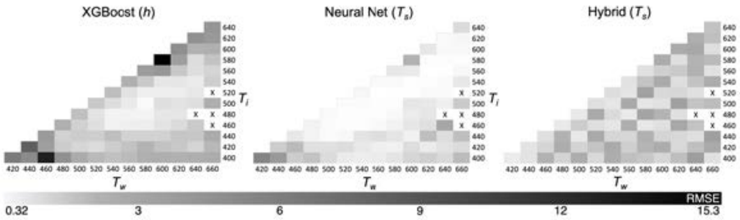
Select Model
Neural Net
XGBoost
Random Forest

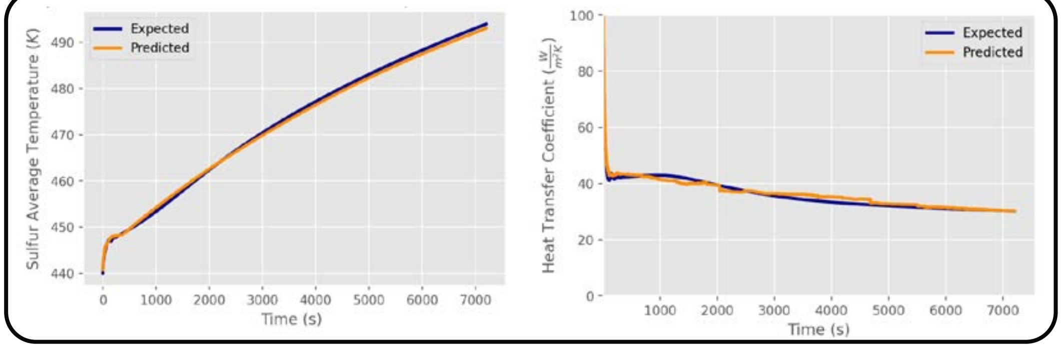
Select Target
Sulfur Avg Temperature
Heat Transfer Coefficient

5-fold Cross Validation
Split Dataset Train / Validation → Train Model ↔ Validate Model → Test Model

Optimize Hyperparameters
Evaluate Results
Refine Model Architecture

Hybrid Model
Train Best Temp (T_s) Model for $t \leq t_\delta$
Train Best HTC Model
Calculate T_s from HTC Predictions and T_s at $t = t_\delta$
Create Hybrid Model Using T_s predictions for $t \leq t_\delta$ and T_s calculations for $t > t_\delta$





Menear, Kevin, et al. No. NREL/CP-2C00-84235. National Renewable Energy Laboratory (NREL), Golden, CO (United States), 2023.
Menear, Kevin, et al. *Sulfur TES ML [SWR-23-02]*. National Renewable Energy Laboratory (NREL), Golden, CO (United States), 2022.

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Thank you!
Questions?

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