

# Developing technology and capabilities to solve MSR off-gas challenges

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# Thank you to everyone that has contributed!

## Colleagues & Contributors

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Reactor analysis: David Holcomb, Brian Riley, Ben Betzler, Scott Greenwood

Thermochemical analysis: Jake McMurray, Abbey McAlister, Dino Sulejmanovic

Thermophysical properties: Dianne Ezell, Ryan Gallagher, Brenda Smith

Spectroscopic analysis: Amanda Lines, Sam Bryan, Heather Felmy, Kristian Myhre, Hunter Andrews

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Salt purification: Kevin Robb, Jordan Massengale, Caleb Redmon

Tritium: Paul Humrickhouse



## Funding

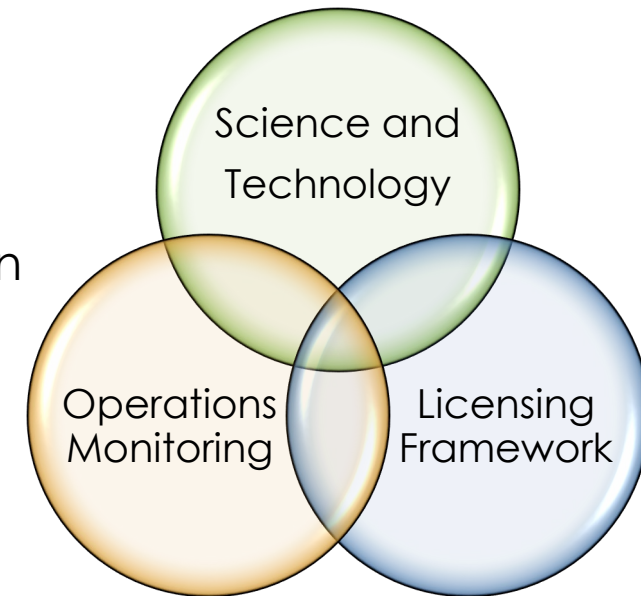
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# The ARC for MSR Technology seeks to facilitate industry success in the deployment of commercial MSRs

- **Approach**

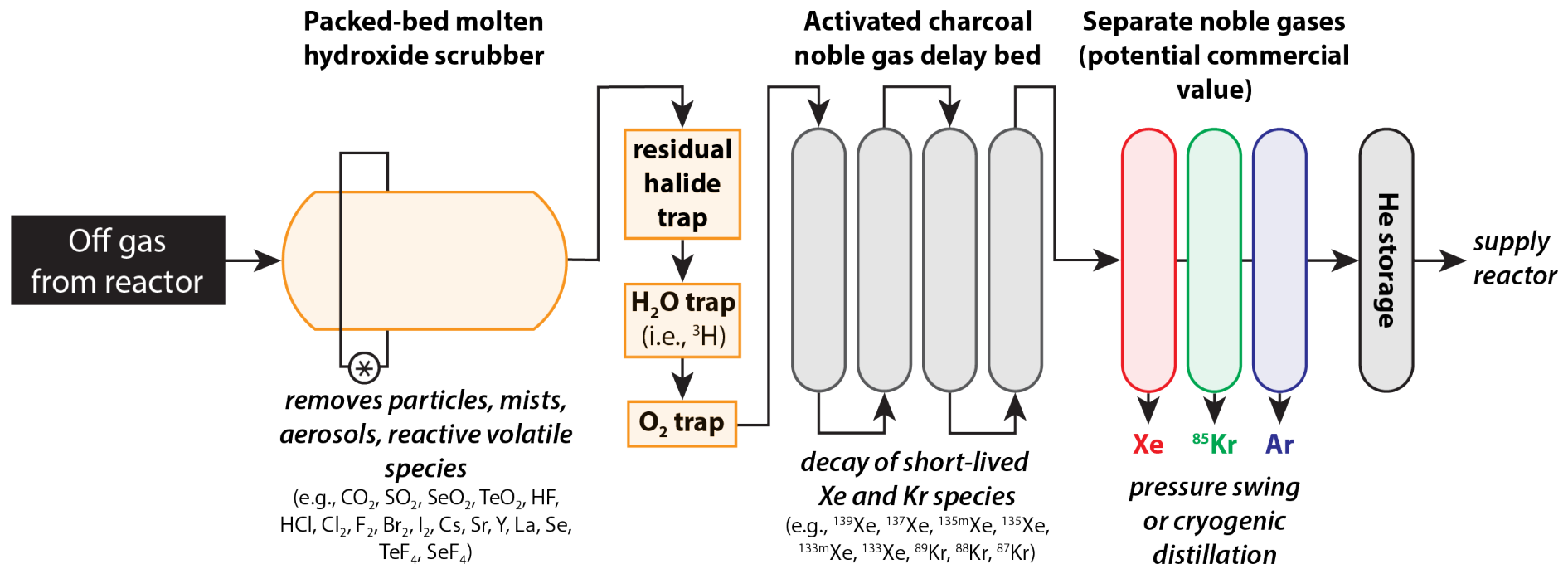
- Understand salt properties, chemical behavior, and transport properties
  - Develop a mass accountancy model for liquid-fueled MSRs
- Study material performance in representative environments
- Develop and demonstrate technology needed for a first reactor
  - **Off gas system technology**
  - Safety assessments and containment strategies
- Develop monitoring capability for first reactors
  - Corrosion potential measurement and localized corrosion detection
  - **Off-gas system species monitoring**
  - In-situ material specimen surveillance



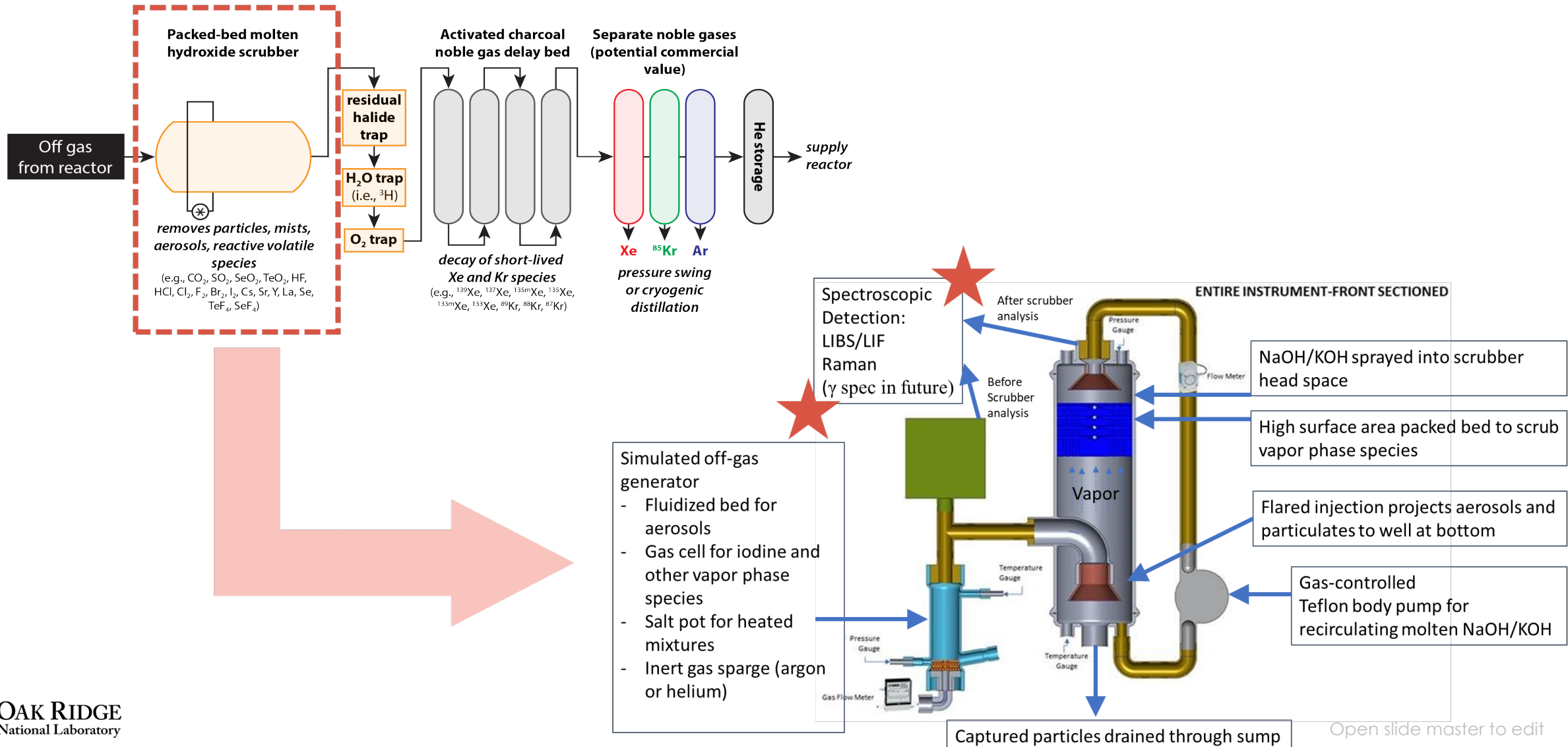


# To support MSR licensing, source term and off-gas challenges need to be addressed

- Design effective off-gas treatment systems for MSRs
  - Thermochemistry tells us what to expect in the salt, cover gas
  - Transport modeling tells us what to expect on surfaces, in porous volumes, and off-gas systems



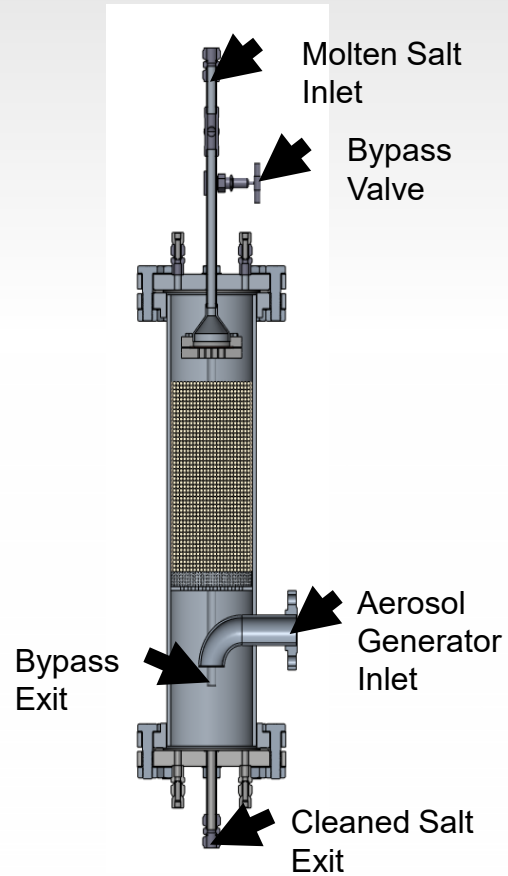
# To support MSR licensing, source term and off-gas challenges need to be addressed



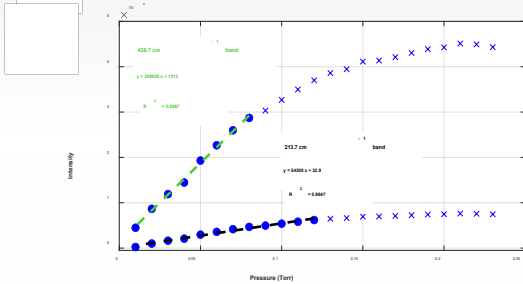
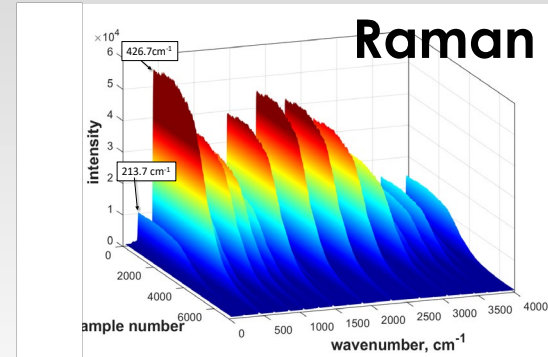
# We are defining functional requirements for an MSR off-gas system.

## Component testing

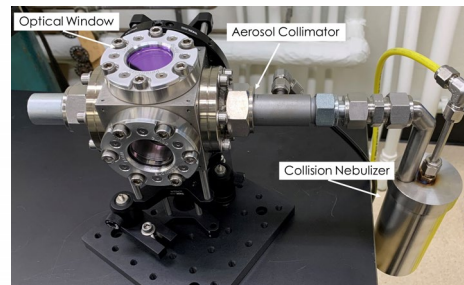
- Molten hydroxide scrubber



## Online sensing

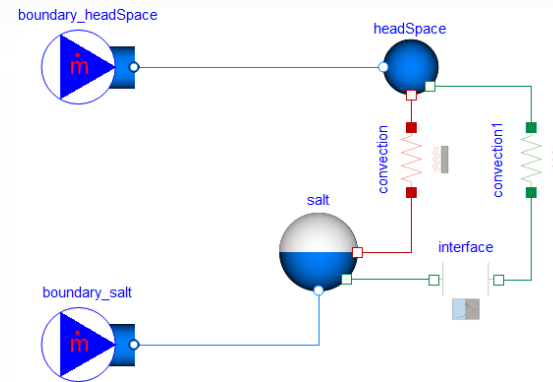


## LIBS



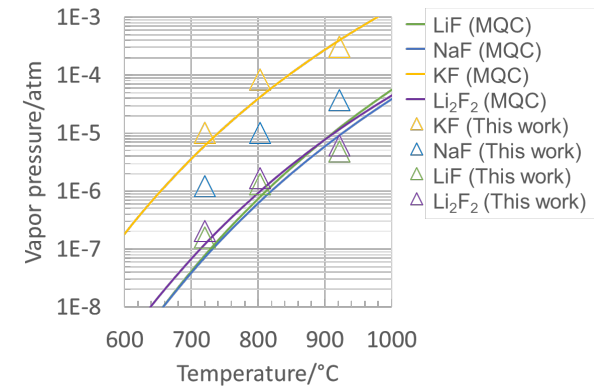
## Systems modeling

- Modeling in Transform
- Mass accountancy
- Gas-liquid interface
- Provides source term to off-gas



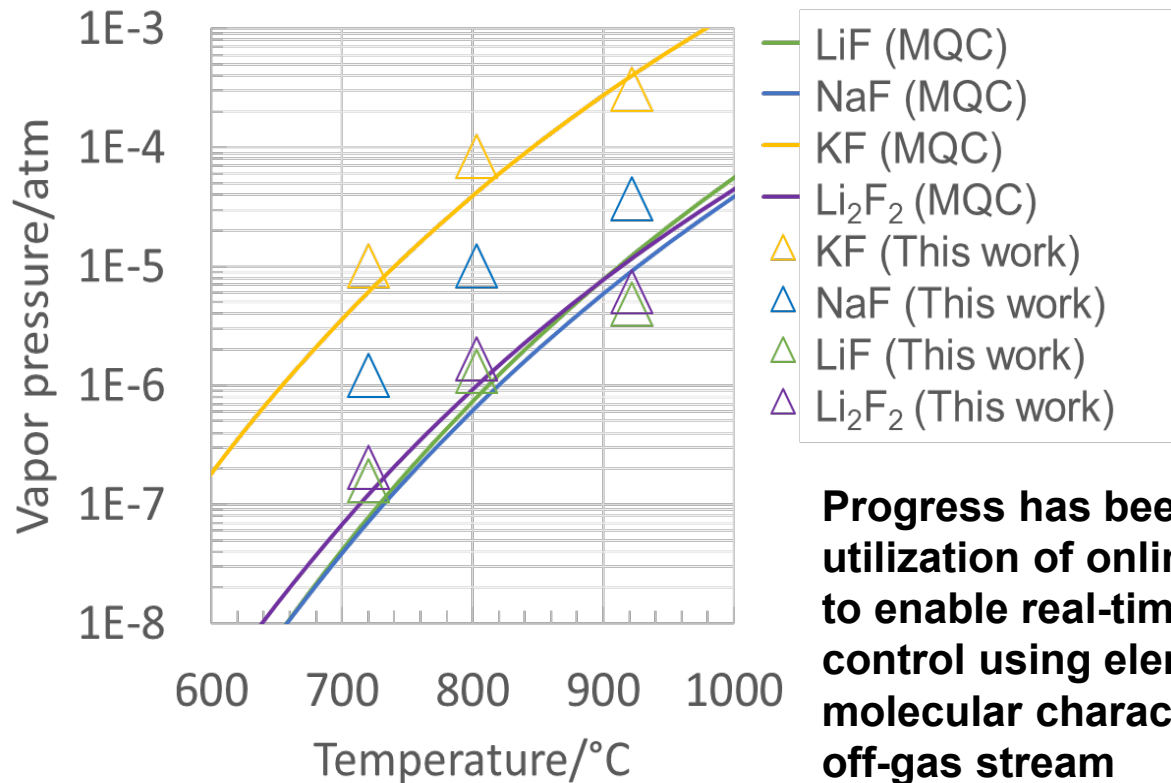
## Coupling with chemical measurements

- Vapor pressures from the Netzsch skimmer will be used to derive evaporation coefficients used in transport models.

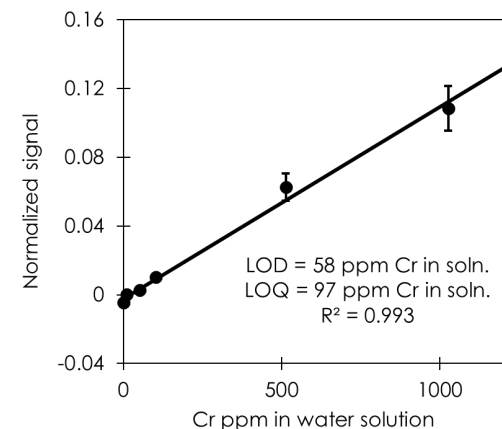
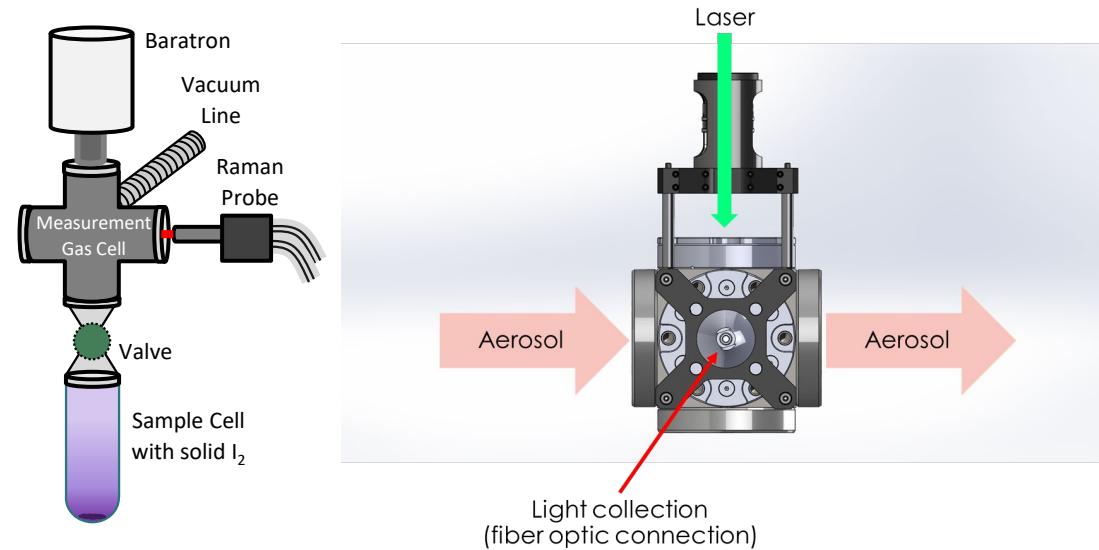


# Off-gas: the intersection of analysis, monitoring, and modeling

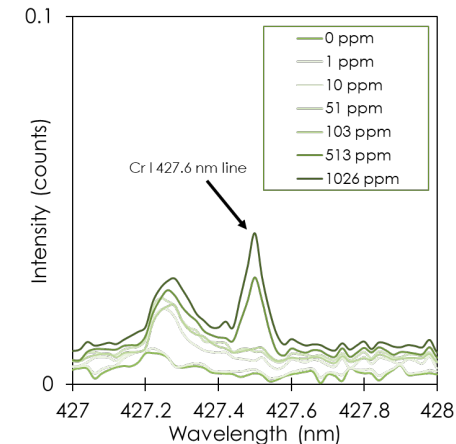
Measurements of vapor pressures over FLiNaK using the Netzsch Skimmer are in good agreement with the computed MSTDB values and can be used for better understanding of off-gas behavior, e.g. mass accountancy modeling



Progress has been made for utilization of online monitoring to enable real-time operator control using elemental and molecular characterization of off-gas stream



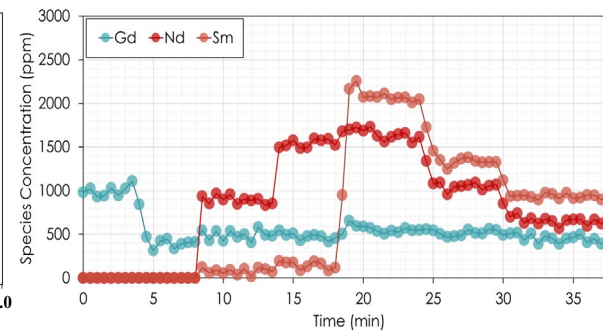
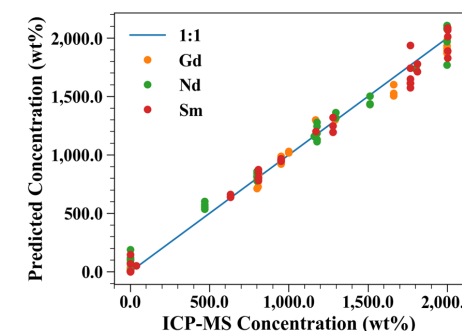
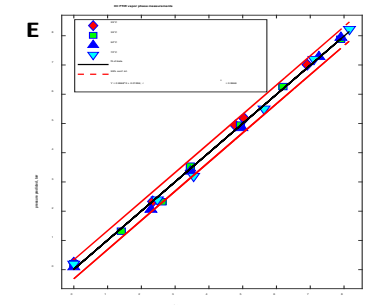
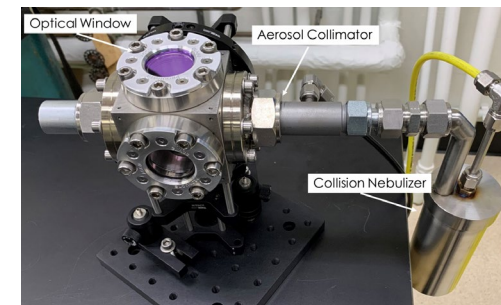
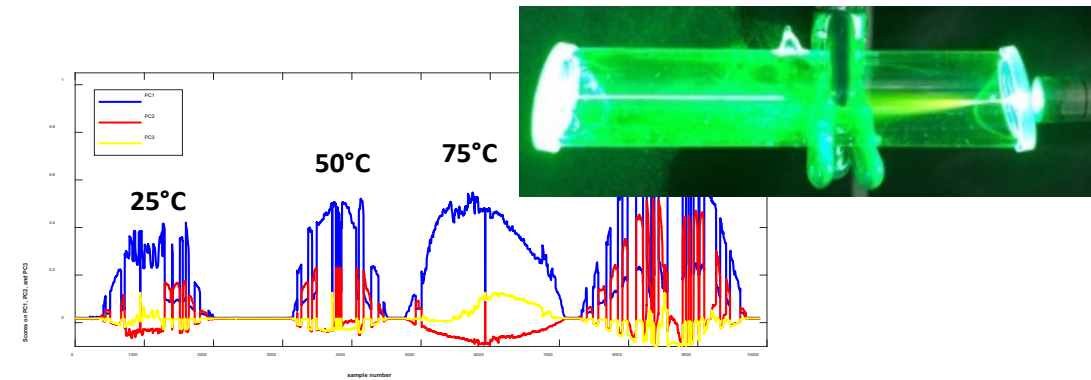
Calibration curve built from Cr I 427.6 nm line



# Online monitoring of off-gas systems performance includes detection of chemical species

- Online monitoring tools are being built and demonstrated to support near-term deployment of MSR systems
- Online off-gas monitoring provides unique insight into reactor performance and allows for efficient and informed operation of off-gas treatment systems
  - The combination of molecular and elemental techniques provides a comprehensive understanding of gas composition
  - Results with Raman and LIBS show optical data can be used to quantify key species within the off-gas

I<sub>2</sub> standard cell illuminated by Raman laser

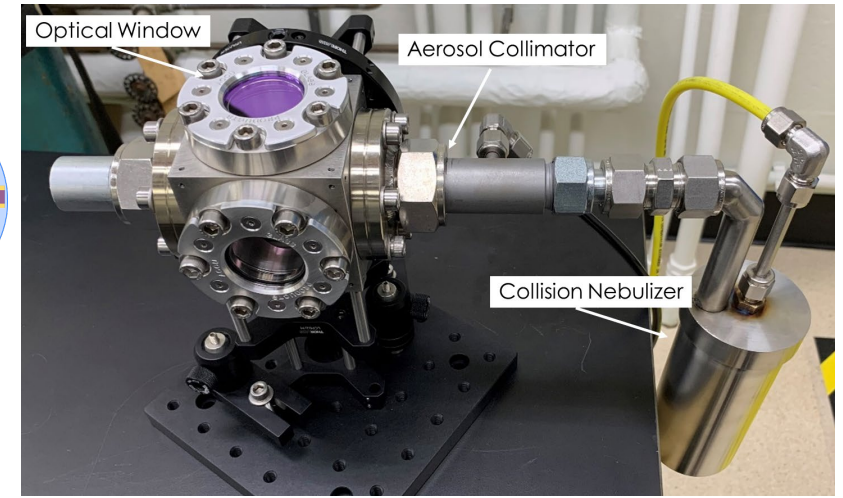
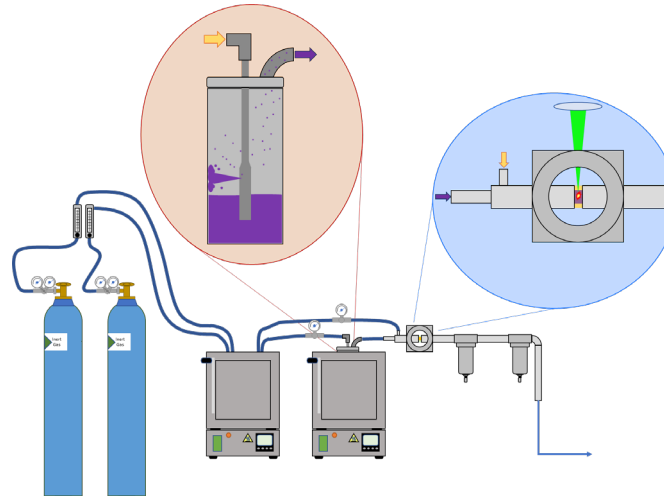




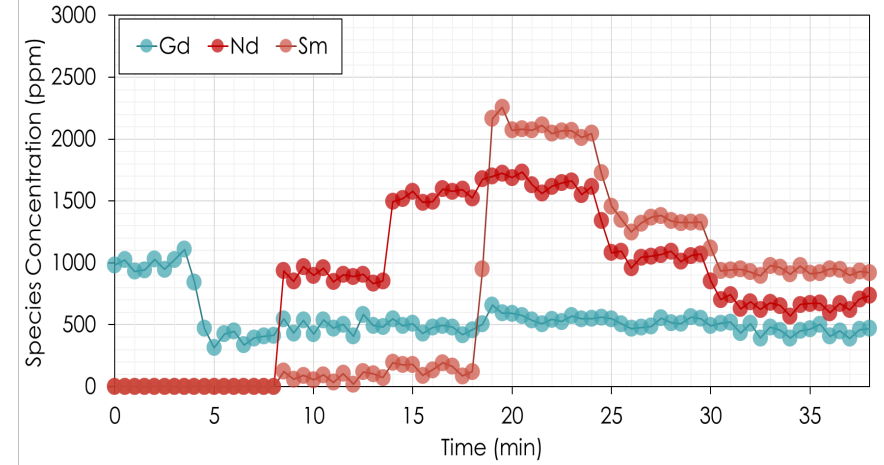
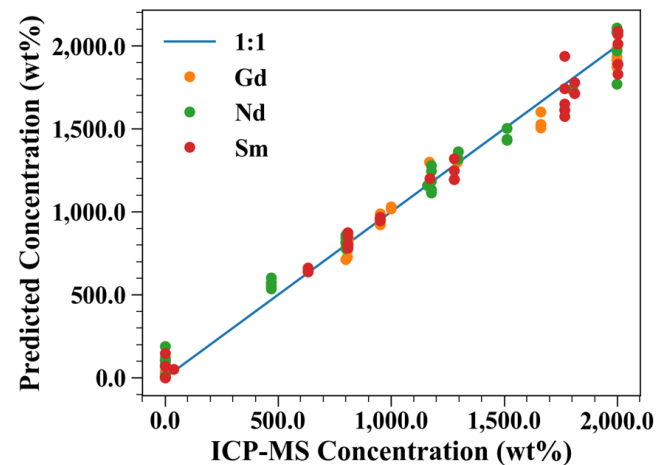
# ORNL: Laser Induced Breakdown Spectroscopy (LIBS)

- Quantitative elemental analysis is important for MSR off-gas
- LIBS was shown to quantify relevant fission product species in aerosols at ppm levels
- Molten salt pot system has been designed and is under construction for testing of online monitoring techniques
- Extension of online monitoring techniques to direct liquid analysis is possible

Conceptual drawing (left) and picture of room-temperature system (right)

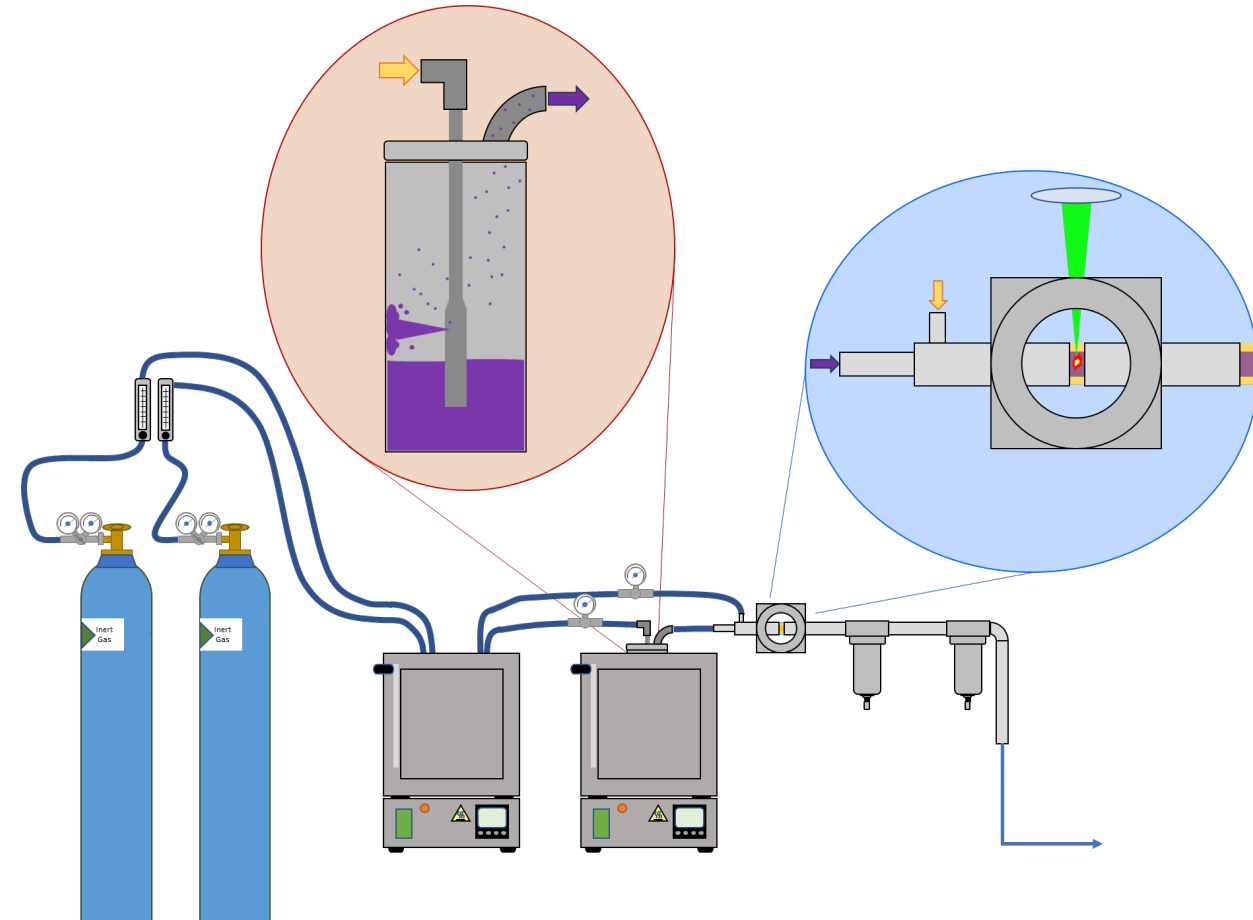


Calibration plot (left) and example real time monitoring data (right)



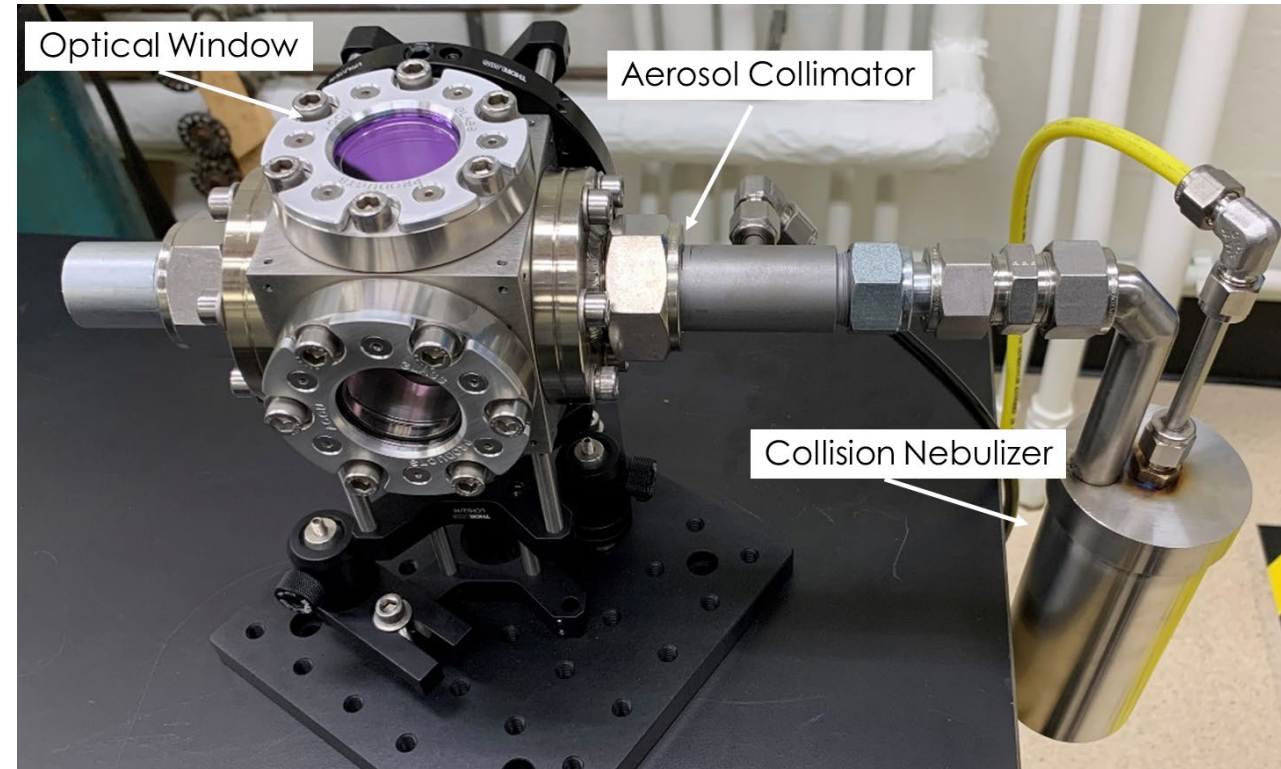
# Laser Induced Breakdown Spectroscopy has been used to provide real-time quantitative elemental information

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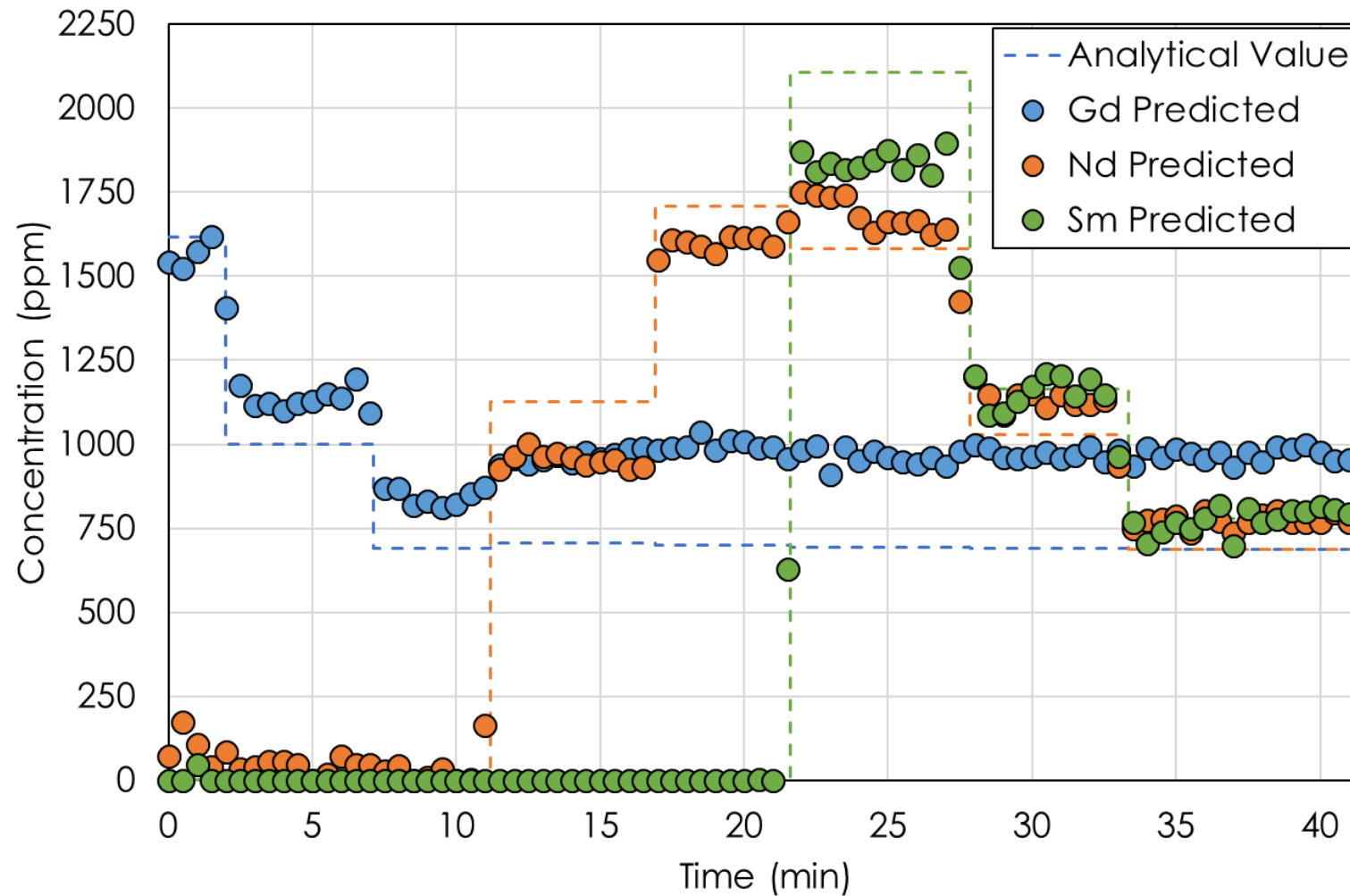


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# Real Time Demonstration – initial concentration predictions

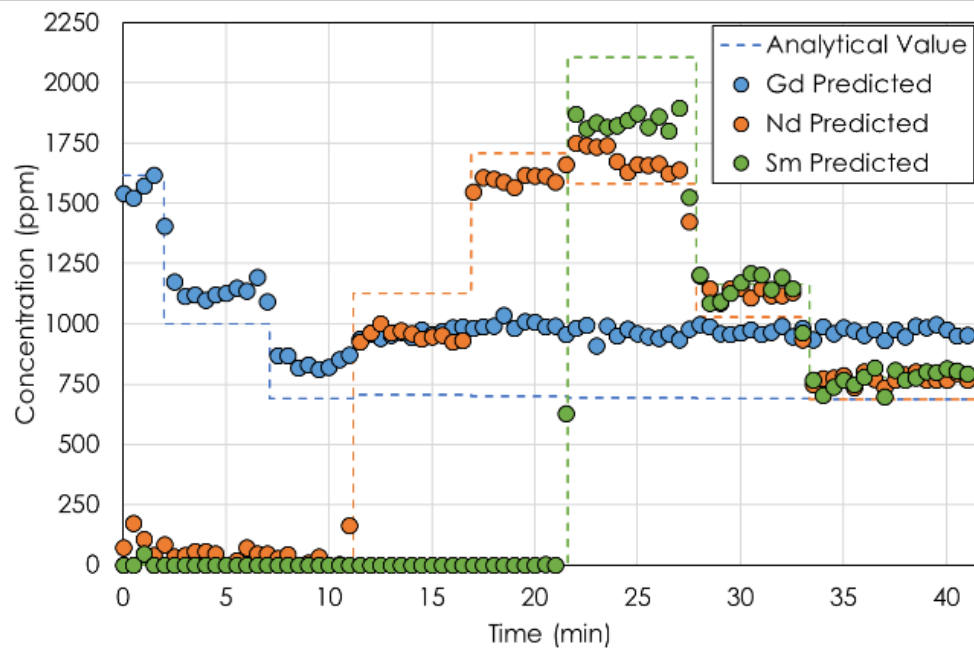




# Machine learning was used to improve accuracy of LIBS analysis

- Advanced optimization algorithms are being explored to dramatically improve predictive analytical models over those achieved using traditional approaches
- A genetic algorithm was used to achieve greatly improved analytical results obtained during real time monitoring of surrogate off-gas streams

### Before Machine Learning Optimizer



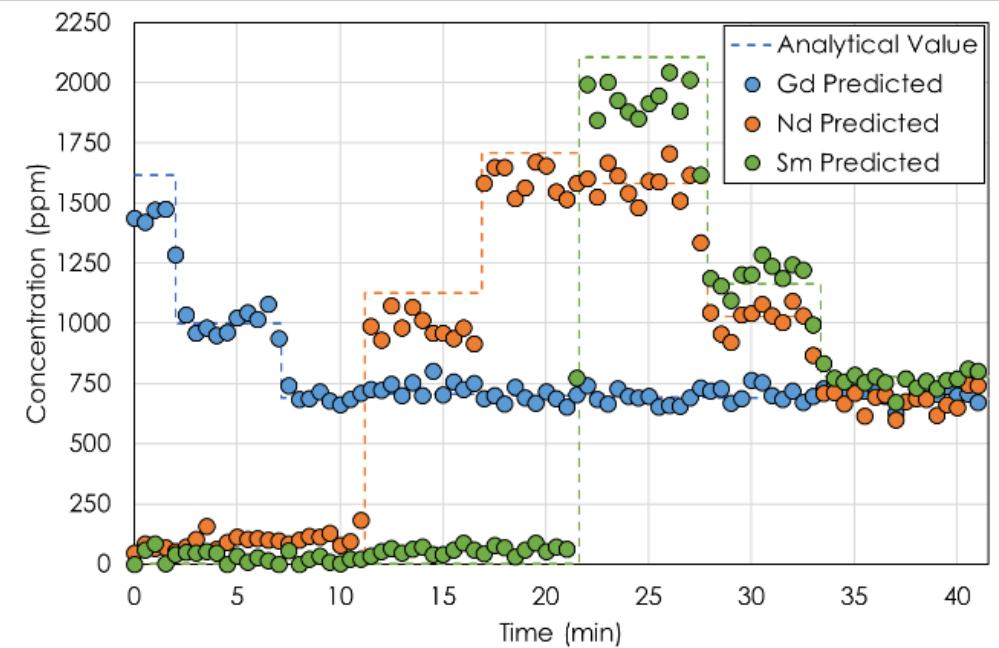
### Error Reduction

Gd  
73%

Nd  
18%

Sm  
25%

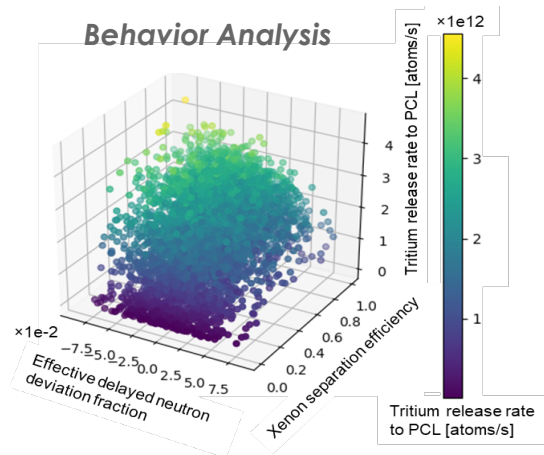
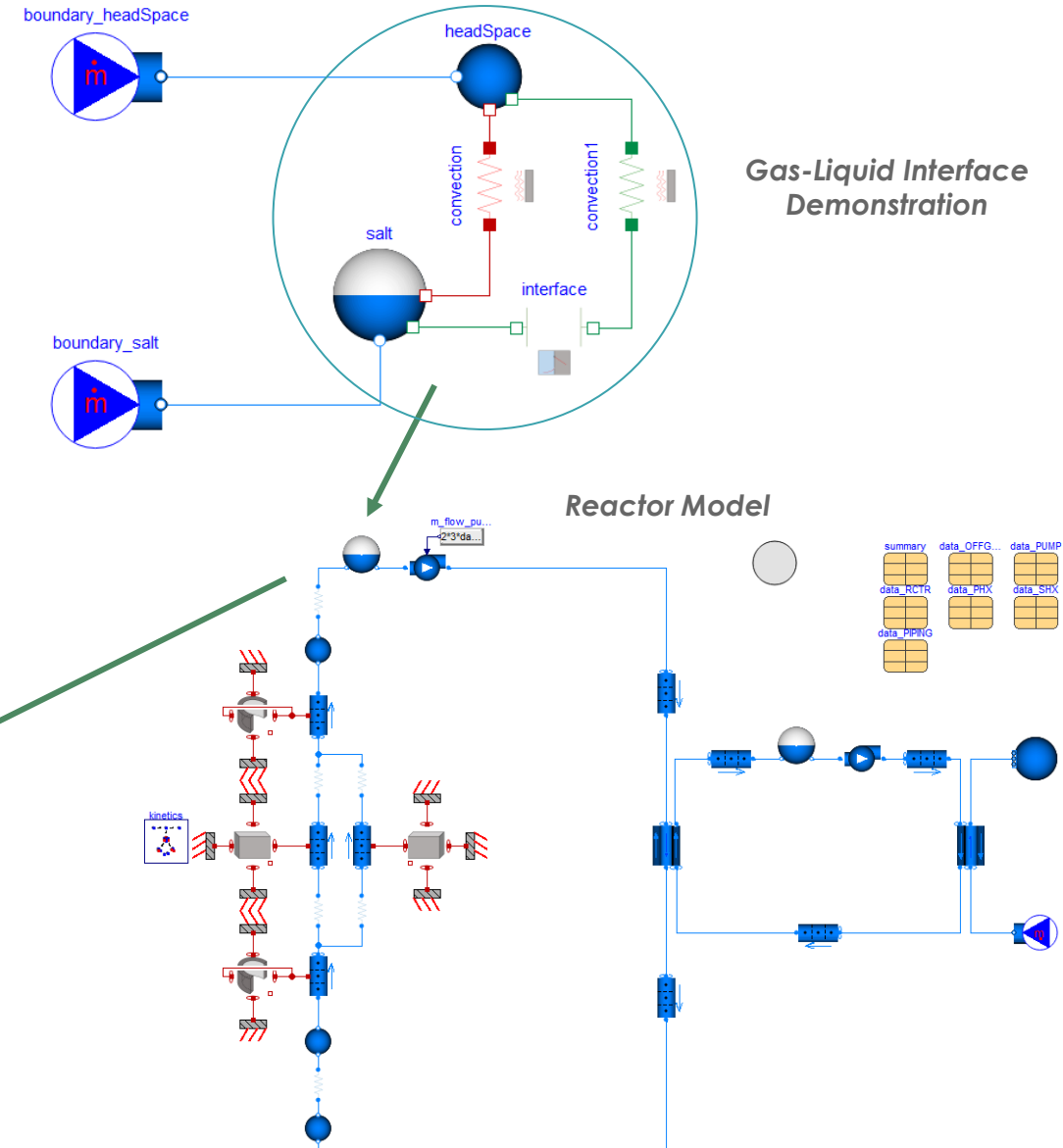
### After Machine Learning Optimizer



# Integrate Experimental Data with Dynamic Simulations

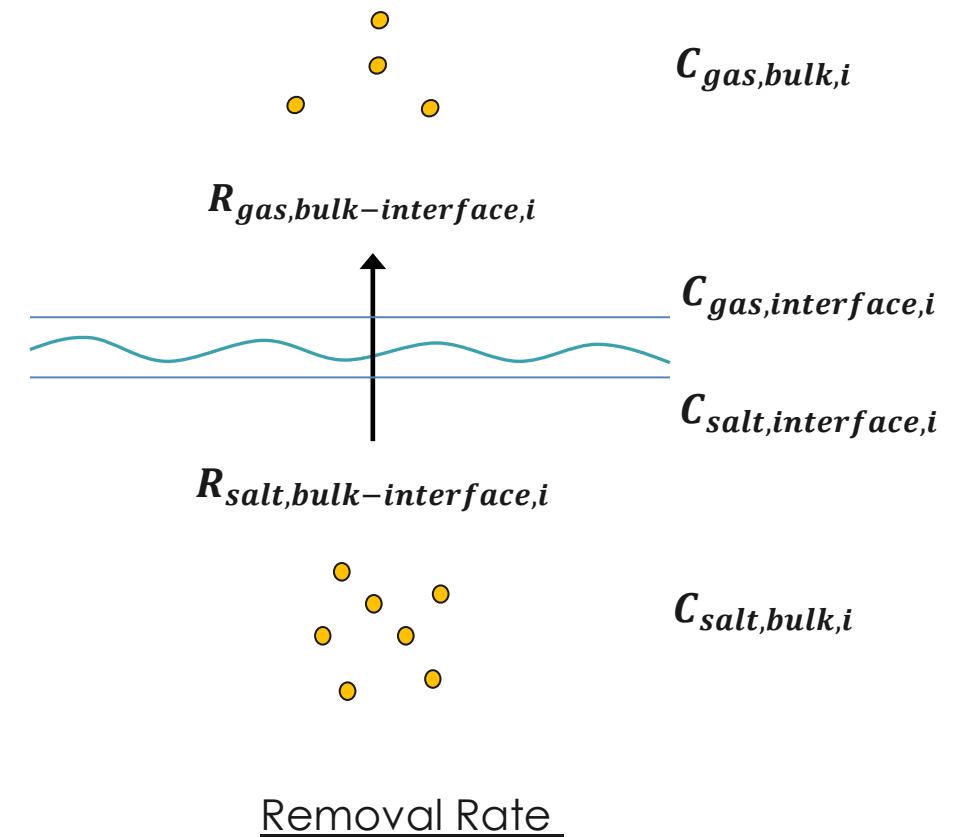
Scott Greenwood, ORNL

- Understand the time-dependent behavior of MSR
- Reactor, off-gas system, and mass transport models
  - Thermophysical Properties | Salt Media Properties
  - Thermodynamic Database (MSTDB)
    - Gas-Liquid Interface Transport – MSTDB Coupling
- Simulation platform (TRANSFORM)
  - Focus on data coupling
  - Enables rapid prototyping
  - Supports radionuclide tracking



# Model demonstration – Salt-to-Gas Interface Transfer

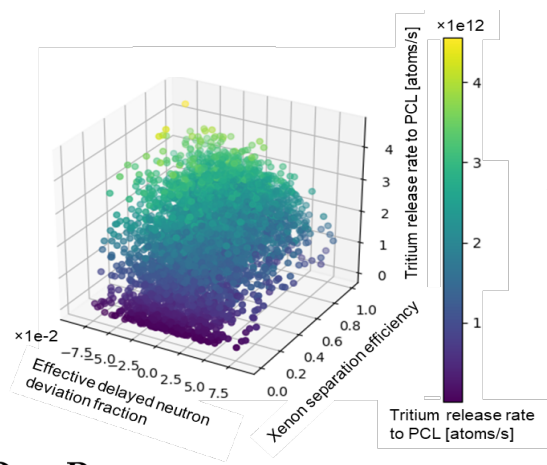
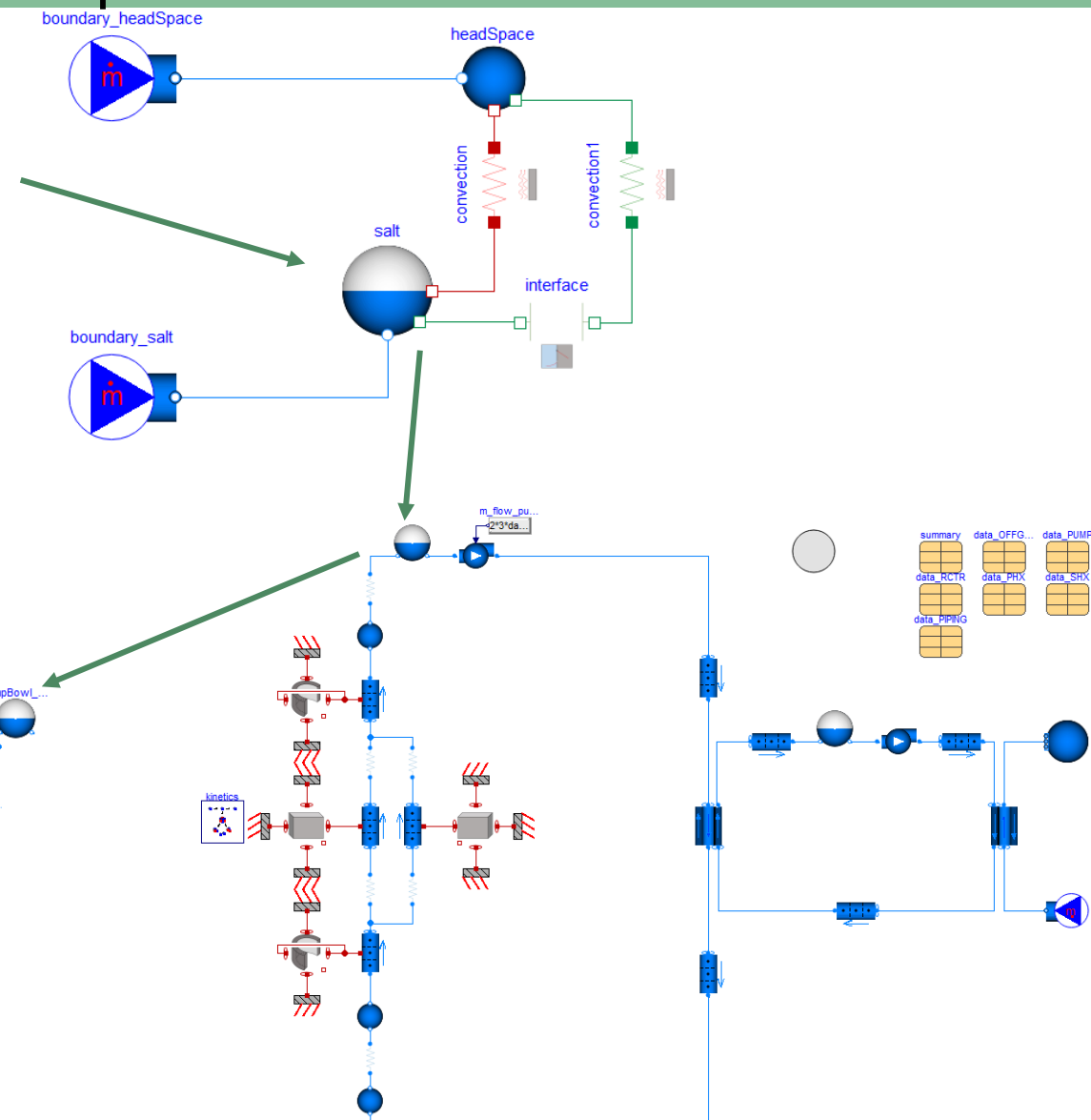
- Salt
  - LiF-NaF-KF-Cs
  - 0.41.85-10.35-37.8-10.0 mol% at time = 0
- Assumptions
  - Closed system
  - Gas phase is pure Nitrogen at time = 0
  - $C_{gas,bulk,i} \ll$  Primary Gas Concentration at all times
  - $C_{salt,bulk,i} = C_{salt,interface,i}$ 
    - i.e.,  $R_{gas,bulk-interface,i} \gg R_{salt,bulk-interface,i}$
  - $C_{gas,interface,i}$  calculated from Thermochemicala
    - i.e., partial pressures based on  $C_{salt,interface,i}$
  - **Inventory in salt is much greater than transferred material**



$$\frac{d(m_i)}{dt} = kA(C_{gas,interface,i} - C_{gas,bulk,i})$$

# Reactor, off-gas system, and mass transport models are integrated into a dynamic system performance code

- Develop mass transfer of representative salt based on physics-based gas-liquid interfaces
- Integrate gas-liquid interface into dynamic molten salt reactor model
- Generate off-gas system model from Campaign design
- Integrate off-gas system into reactor model





# Big takeaways...

- Source term and off-gas challenges need to be addressed to support licensing of MSR
- An ORNL-led multi-institution collaboration is establishing capabilities and developing technologies to address these source term and off-gas challenges
  - Technologies: treatment systems, sensors (LIBS, Raman, etc.)
  - Capabilities: system modeling tools, experimental test stand
- Sensor technologies can be extended to direct salt analysis



# Questions?

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