

Nuclear **S**cience, **T**echnology and **E**ducation for **M**olten Salt Reactors (**NuSTEM**):

Project overview and recent advances

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MSR Workshop, Oct. 14, 2020

Background on NuSTEM

- **Grand Challenge Problem for Nuclear Energy (IRP-NE-1 in FOA for FY 2017)**
 - *Need for new specialists to become engaged in the nuclear technology field*
 - Grant as a prototype of DOE's international engagement within the **OECD/NEA's NEST (Nuclear Education, Skills and Technology) Framework**

DOE signs Gen-IV MOU
on MSR, Jan. 2017

Pursuant to Section 7 of the Generation IV International Forum Memorandum of Understanding for Collaboration on The Molten Salt Reactor System Nuclear Energy System under which cooperation began on 6 October 2010 between the COMMISSARIAT A L'ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES and the EUROPEAN COMMISSION JOINT RESEARCH CENTRE, and to which ROSATOM and the PAUL SCHERRER INSTITUTE subsequently became Participants on 12 November 2013 and 20 November 2015 respectively, the UNITED STATES DEPARTMENT OF ENERGY is a new Participant from the date of signature hereunder:

FOR THE UNITED STATES DEPARTMENT OF ENERGY:



Ray Furstenau

Associate Principal Deputy Assistant Secretary
for the Office of Nuclear Energy

Date: 5 January 2017

Place: Washington, DC

- **NuSTEM's goals:**
 - To deliver science and results for the **advancement of molten salt reactors**
 - To **train/educate the next generation of molten salt reactor experts**

NuSTEM : Areas and Team Overview

Five research tracks:

1 Data and System Evaluation:

1.a *Modeling and Simulation*



Ragusa



Fratoni



Tsvetkov

1.b *Cross-section measurements*



Batchelder



Bernstein

1.c *Thermal-hydraulics*



Kimber



Kurwitz

2. Material/corrosion science:



Shao



Couet



Sridharan

3. Chemical Technology (Sensors and Waste Forms)



Scarlat



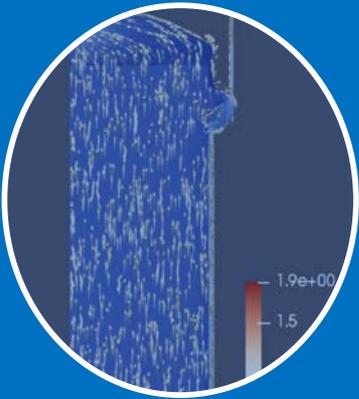
McDeavitt



Ortega

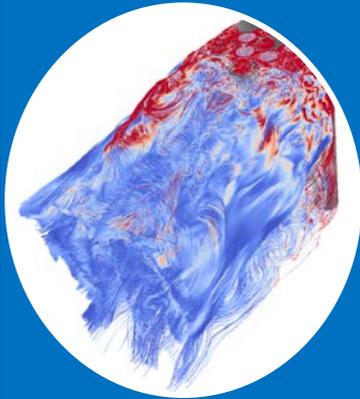
One educational track

NuSTEM thrusts



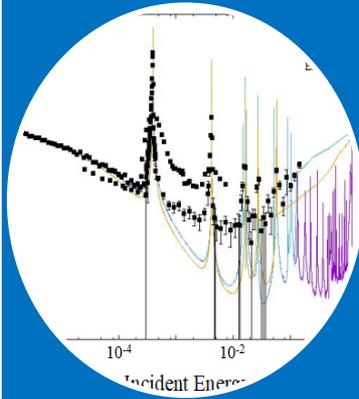
Modeling and simulation

- Development of tools / models for phenomena specific to MSRs
- Application of Data Science for rapid design optimization and uncertainty quantification
- System performance



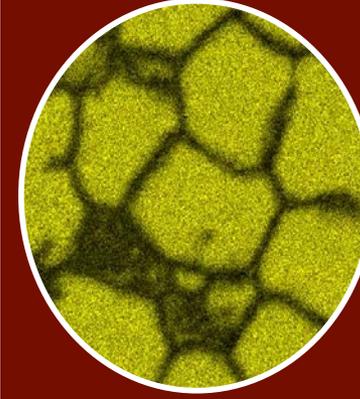
Thermal-hydraulics

- V&V of computational CFD models
- Investigation of passive heat removal using heat pipes



Cross section

- Measurement of $Cl-35$ (n,p) cross section reaction in the fast spectrum range



Materials and corrosion

- Corrosion testing with unirradiated and irradiated alloys
- Material characterization and optimization

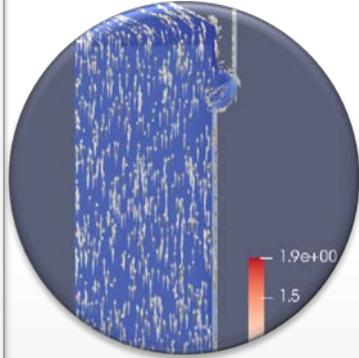


Chemical Technologies

- Development and demonstration of chemical and thermal sensors
- Sensor prototype built
- Manufacturing methods and materials for probe
- Waste stream characterization

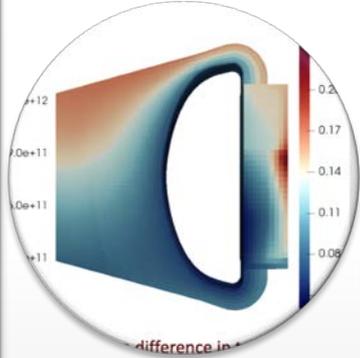
Education and training: development of human capital and expertise

Data, Modeling & Simulation Thrusts



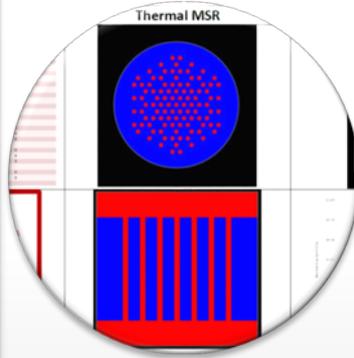
High-fidelity modeling

- Multiphysics model with Monte Carlo + CFD
- Reference solution



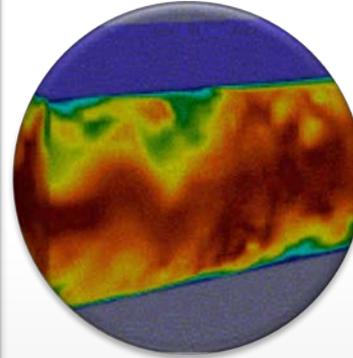
Reduced-order models (ROM)

- Develop ROM for multi-physic simulations of MSRs
- Transient analysis and UQ using ROMs



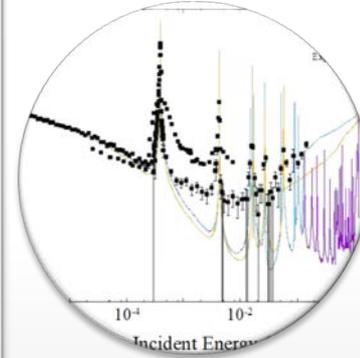
System analysis

- Evaluate MSRs' long term operation
- MSR lifecycle assessment



Thermal-hydraulics

- Assess validity of applying LWR flow predictions
- Develop transient and steady state models for heat pipes



Cross sections

- $\text{Cl-35}(n,p)$ cross section the fast energy range

Enabling technologies for the design, analysis, and optimization of MSRs

Objectives:

- MSRs have unique features that traditional codes cannot handle (e.g., delayed neutron precursor drift, salt compressibility).
- No or limited experimental data available (e.g., MSRE).
- Highly accurate models capable to represent the unique features of MSRs can improve our understanding of MSRs and can provide benchmark data for simpler model until experimental data will be available.

Approach:

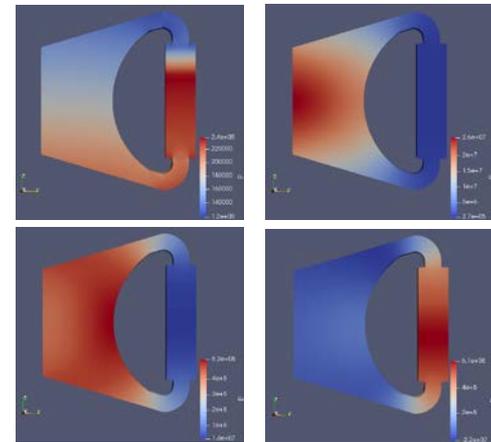
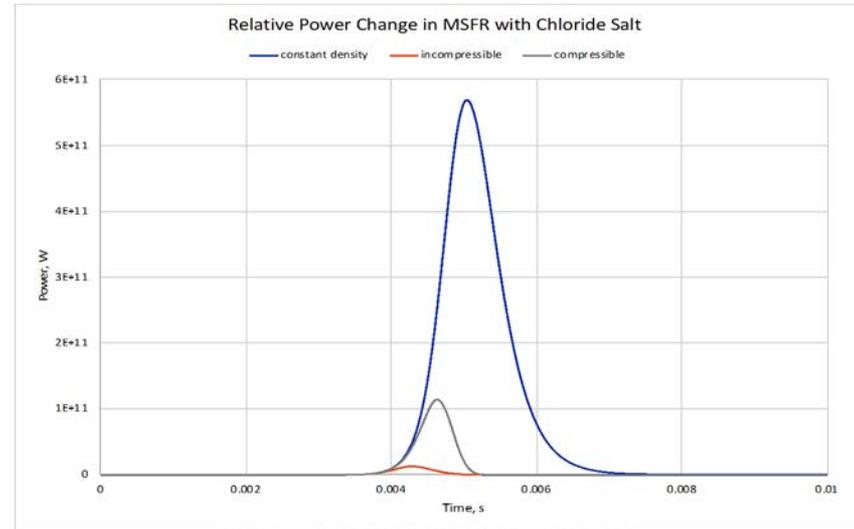
- Use of Monte Carlo code (Serpent) for neutronics and the OpenFOAM toolkit (specifically the GeN-FOAM library) for thermal-hydraulic.
- Use data from the MSRE when possible as benchmark.

Key Findings:

- The GeN-FOAM library for successfully expanded to include adjoint solver and other components functional to MSR modeling
- Delayed neutron precursors behavior was successfully implemented in thermal-hydraulics and neutronics calculations and benchmarked against MSRE data.
- The impact of salt compressibility during accident scenarios (reactivity initiated accidents) evaluated in coupled simulations.

Impact

- Phenomena unique to MSRs are modeled with the smallest number possible of assumptions
- Improved understanding of MSRs behavior such as importance of salt compressibility
- Data generation for training Reduced Order Models (next slide)



Pressure change during a RIA with chloride salt when accounting for compressibility at $t = 0, 4E-3, 5E-3, \text{ and } 6E-3$ s.

Objectives:

- High-fidelity simulations for MSRs are challenging:
 - Additional physical phenomena compared to LWRs
 - Reliance on first-principle simulation tools (CPU demanding)
 - Thus, any multi-query problem (e.g., design optimization or uncertainty quantification) will be expensive.
- Data Science techniques to learn input-output behaviors of high-fidelity models, under parametric variations.

Approach:

- Model order reduction can significantly lower the computational complexity of such simulations:
 - Deriving low-dimensional representation of complex systems
 - This yields a drastic reduction of the model's number of unknowns.
- Selected technique: Method of Snapshots + Proper Orthogonal Decomposition (POD) + Galerkin-projection of full-order model

Key Findings:

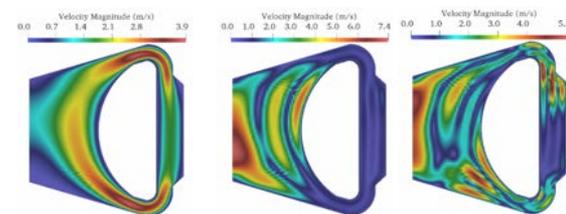
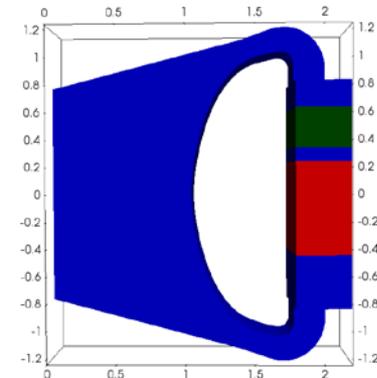
- Model order reduction is very effective.
- It can be adapted in DOE and industry codes (e.g., black-box codes).

Impact

- Extension to **parametric** problems (crucial for design optimization + UQ) and noted large speedups.
- One of the first applications of reduced-order models to multi-group **criticality** problems; to **RANS in laminar+turbulent flows**, and to **multiphysics simulations** applied to **MSRs**.

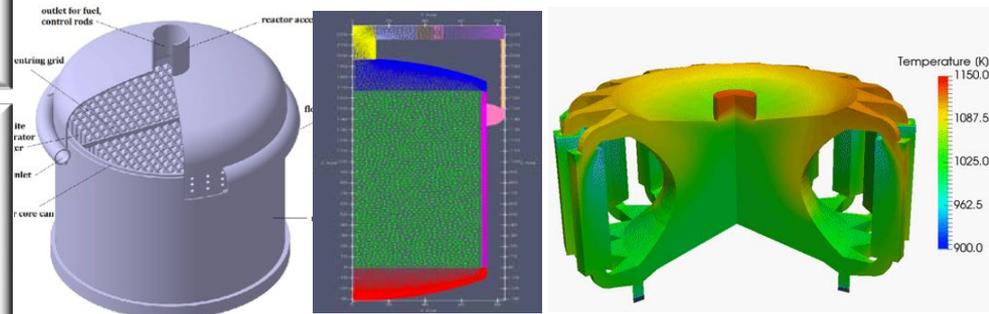
Reduced order modeling for UQ: *steady-state flow in the MSFR in routine operation*

fluid viscosity $\in [0.1,1.0] \text{ m}^2/\text{s}$
 pump strength $\in [1.0,3.0] \text{ N}/(\text{m}^3\text{s})$



Mean L^2 -error velocity (%)	Max L^2 -error velocity (%)	Mean L^2 -error pressure (%)	Max L^2 -error pressure (%)
0.53	0.76	0.17	0.58

A reduced-order model using ~ 10 modes can **speed up** simulations by a **factor of 4000**



Objective:

- The focus of the task is to develop capabilities and evaluate performance of MSRs accounting for operational dynamics under assumptions of sustainable long-term operation with minimized environmental impact

Approach:

- Peculiarities of Circulating Fuel Reactors in reactor physics simulations accented for through integration of scripting and high-fidelity models to yield an integral performance model
- Dynamics system model with DNP drift coupled to the reactor model for fuel cycle and environmental evaluations
- Accounting for salt properties within the MSR modeling framework through salt property databases and data catalogs

Key Findings

- Evaluations of the MSR operational characteristics and parametric studies of select metrics demonstrate and quantify adaptability of MSRs
- Evaluation of MSRs focusing on sustainability metrics
- Formulation of the MSR lifecycle analysis approach and exploration of the current design space

Impact:

- MSR system-level modeling framework based on Serpent modeling capabilities targeting fuel cycle and resource evaluations
- Environmental impact analysis of the MSR lifecycle from construction to decommissioning
- Design space evaluation to assess and optimize the resource utilization assuming deployment of MSRs

Synthesis

$$\bar{\mu} = Y_{\mu} \exp\left(\frac{Z_{\mu}}{T}\right) \text{ Reduced viscosity}$$

Mixing Rule for Potential Parameters

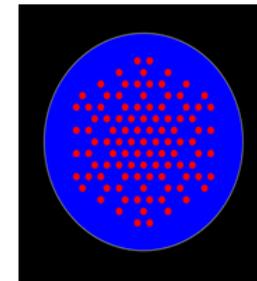
$$Y_{\mu} = (1 - x_2)^2 Y_{\mu,1} + (1 - x_2)x_2(Y_{\mu,1} + Y_{\mu,2}) + x_2^2 Y_{\mu,2}$$

$$Z_{\mu} = (1 - x_2)^2 Z_{\mu,1} + (1 - x_2)x_2(Z_{\mu,1} + Z_{\mu,2}) + x_2^2 Z_{\mu,2}$$

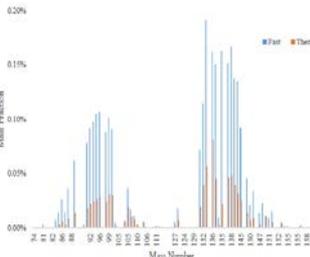
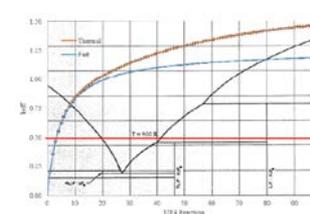
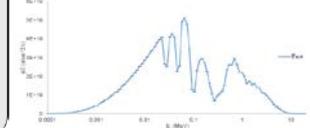
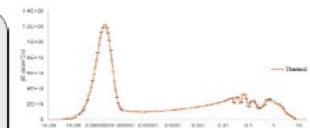
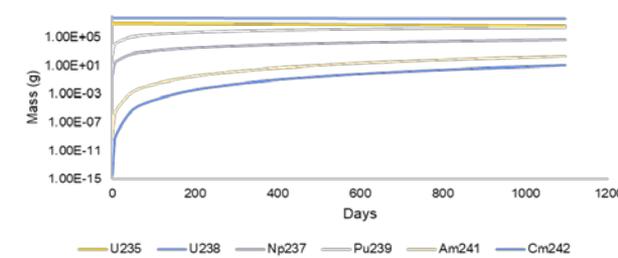
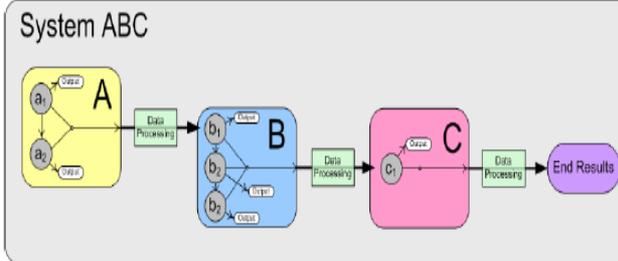
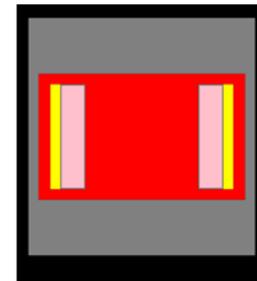
Green-Kubo Model

$$\eta = \frac{V}{k_B T} \int_0^{\infty} \langle \sigma_{\alpha\beta}(0) \sigma_{\alpha\beta}(t) \rangle dt$$

Thermal



Fast



	MSFR	MOL	EOL
H3		211.23	826.98
Kr83		1061.08	4089.89
Xe135		64.37	65.63

Objectives:

- Identify flow scenarios in need of validation and analyze uncertainty propagation of turbulence models and material properties.
 - a) High fidelity turbulence modeling not feasible for reactor scale physics (especially any coupled physics)
 - b) No validation grade data available for lower fidelity approaches

Approach:

- Conduct RANS-based simulations and compare to existing experimental data.
- Perform DNS (numerical experiments) of key flow scenarios, as needed.

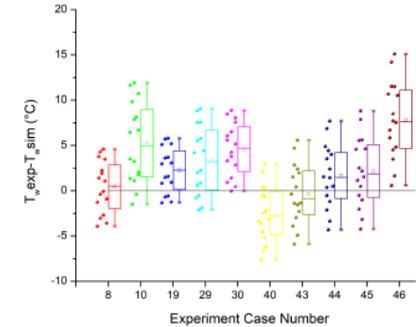
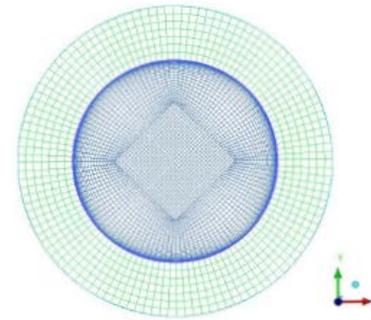
Key Findings:

- Available data for turbulence modeling validation efforts either lacks required statistical metrics or is confounded by large uncertainty in material properties.
- Salts can be considered as Newtonian fluids with excellent agreement to existing correlations for fully developed flow.
- Turbulence modeling for developing flow conditions shows high variation depending on model chosen.

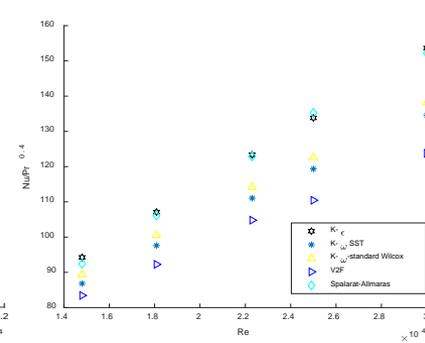
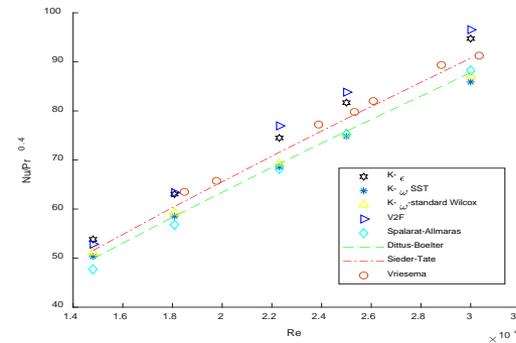
Impact

- Considering families of RANS-based turbulence models for canonical flow geometries provides insight into aspects of flow physics most important to quantify.
- Performing DNS of similar configurations enables a more robust assessment of those RANS-based approaches.

Impact from Material Properties Uncertainty



Fully Developed and Developing Flow



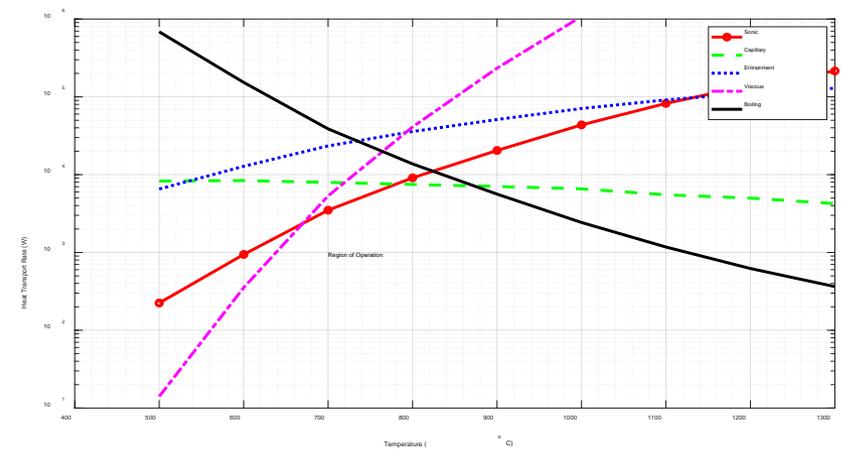
- Objectives:**
- Identify key applications in typical MSR environment where heat pipes find merit
 - Create open-source design tool for passive thermal management in MSRs via heat pipe technologies.
 - Heat pipes have a history in nuclear reactor, but are typically restriction to low thermal power or space applications.
 - Existing tools are typically proprietary or lack capabilities important in MSRs

- Approach:**
- Create 0-D and 1-D lumped models for heat pipes (steady and transient) for near-term implementation in DOE codes.
 - Create 2-D finite volume heat pipe modeling capabilities.

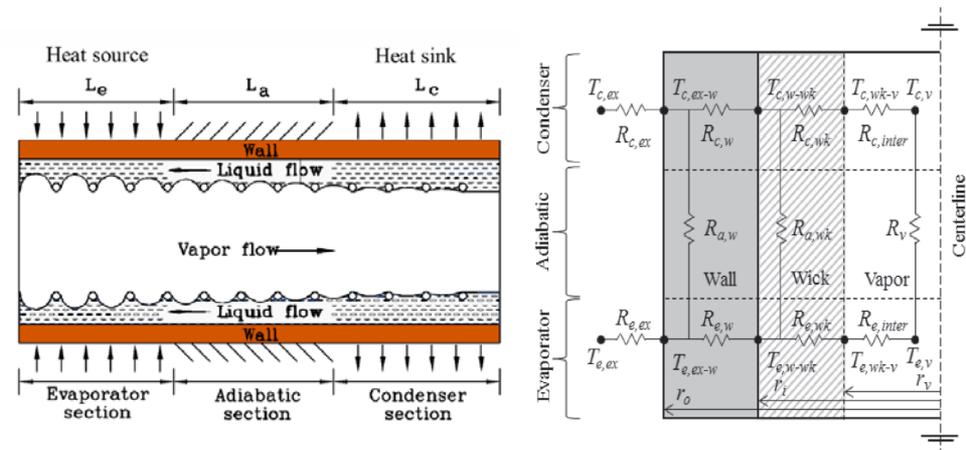
- Key Findings:**
- Performance enhancement could be made in applications involving heat transfer from drain tank and/or containment by implementing heat pipes.
 - 0-D and 1-D models are straightforward, but open-source 2-D finite volume requires additional effort.

- Impact**
- Simplified 0-D and 1-D lumped models enable efforts focused on implementation into DOE codes
 - Open-source efforts (lumped and FV approaches) provide broader impact for future heat pipe-based design efforts in MSRs

0-D Performance Limits



Transient and Steady State Models



Objectives:

- High-purity level of Cl-37 for MSR fast-spectrum application is driven by the current knowledge in Cl-35 cross sections.
- However, the faster energy range for $^{35}\text{Cl}(n,p)$ and $^{35}\text{Cl}(n,\alpha)$ has not been thoroughly investigated .

Approach:

The $^{35}\text{Cl}(n,p)^{35}\text{S}$ and $^{35}\text{Cl}(n,\alpha)^{32}\text{P}$ reactions were measured using quasi-monoenergetic neutrons from the High Flux Neutron Generator (HFNG) at UC Berkeley.

- The cross-section for $^{35}\text{Cl}(n,\alpha)$ agrees somewhat well with ENDF calculations.
- The $^{35}\text{Cl}(n,p)^{35}\text{S}$ cross-section is much lower than the ENDF/B-VII value.
- Structure is observed in the $^{35}\text{Cl}(n,p)$ reaction, consistent with a previously observed level at 11.24 MeV.

Key Findings:

- This finding highlights the need for additional energy differential measurements to better understand reactions in this intermediate energy region.

Impact

The results have been published in Physical Review C, and input into EXFOR is in process.

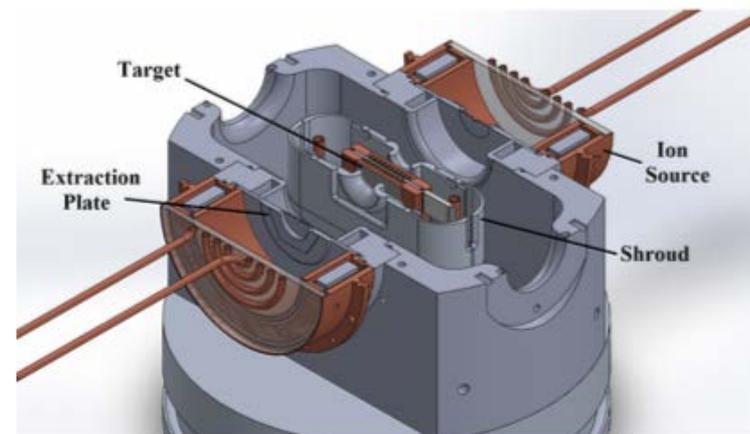
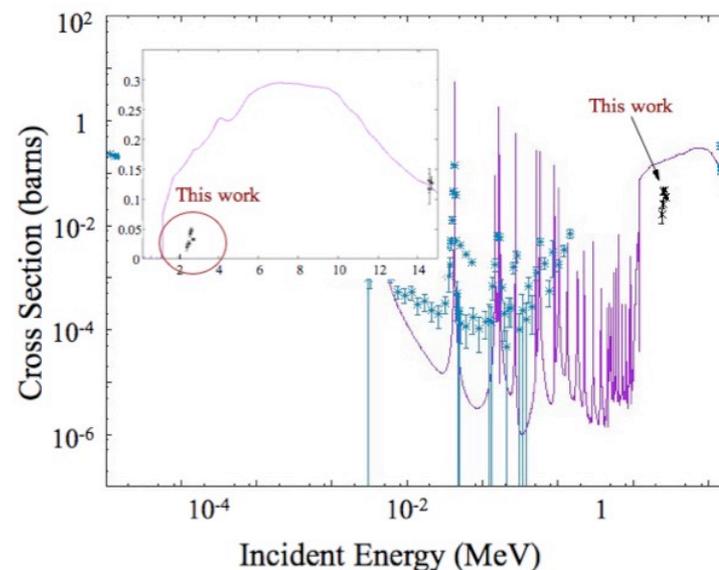
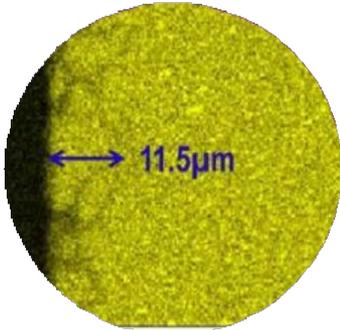


Figure 1. Cut-away schematic of the HFNG. The ion source is approximately 20 cm in diameter.

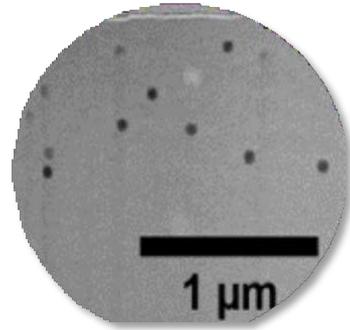


Materials Irradiation and Corrosion Science



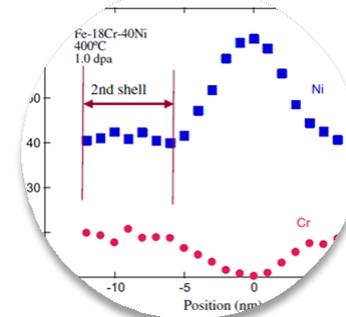
Corrosion Evaluation of Hastelloy-N

- Characterization of corrosion resistance in well controlled conditions
- Corrosion resistance in uranium bearing salts
- Demonstrate in-situ corrosion monitoring



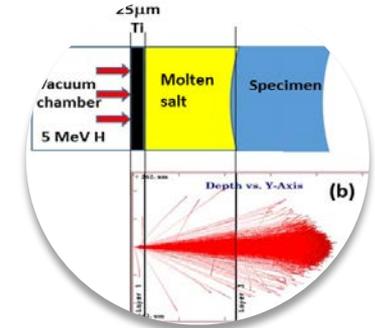
Void swelling study

- Irradiation resistance behavior of Hastelloy-N, A709, and 316SS at very high dpa using ion irradiation
- Simultaneous helium injection and self ion irradiation damage



Synergistic effect of corrosion and irradiation

- Effect of pre- irradiation on corrosion resistance of Hastelloy-N
- Focus on radiation induced segregation
- Cover larger experimental matrix for separate effects



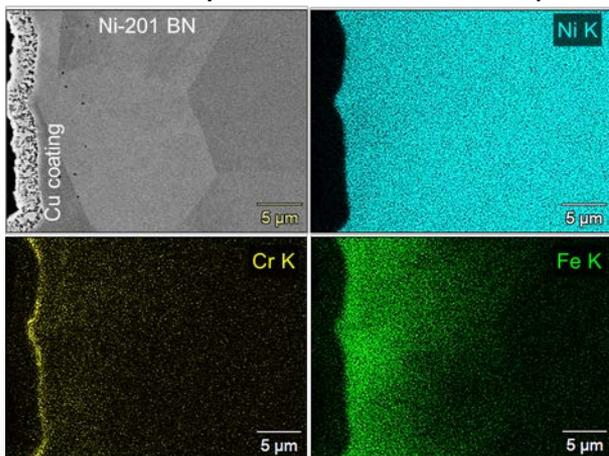
Coupling of corrosion and irradiation

- In-situ irradiation effects on corrosion
- Radiation effect on surface corrosion mechanism
- Steady state behavior representative of MSR

Enhance the understanding of materials performance in MSR environments

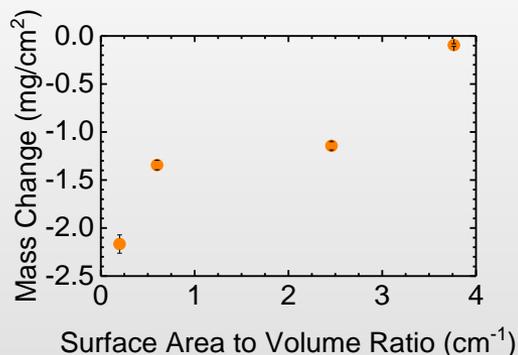
Corrosion Environment Interactions

- Dissimilar Material Interactions
 - Activity Gradient Mass Transport



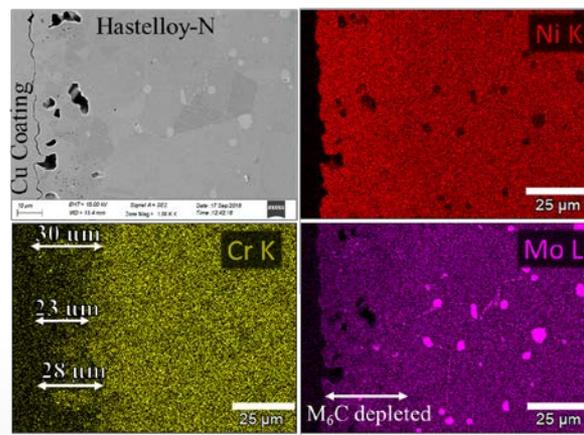
Falconer et al. 2020

- Effects of Salt Volume

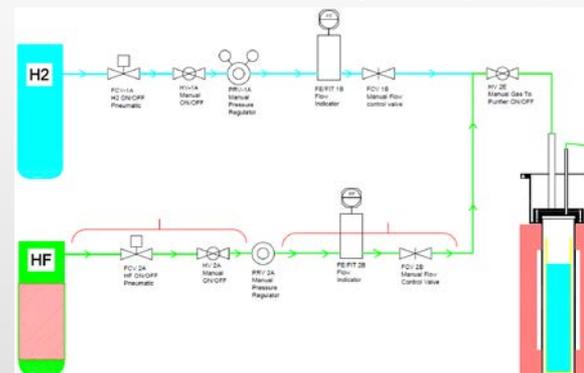


Corrosion Evaluation of Hastelloy-N

- Characterization of corrosion resistance in controlled conditions



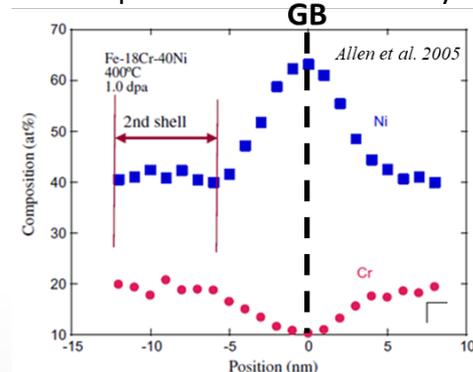
- Salt Purification to improve quality



Synergistic effect of corrosion and irradiation

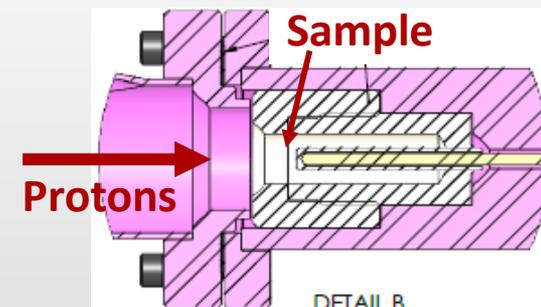
- Effect of pre-irradiation on corrosion resistance

Example of RIS in Fe-Cr-Ni alloy



Cr segregation due to radiation

- In-situ irradiation and corrosion on commercial alloys



Objectives:

- Identify key factors which determine corrosion and irradiation resistance and their synergistic effects

Approach:

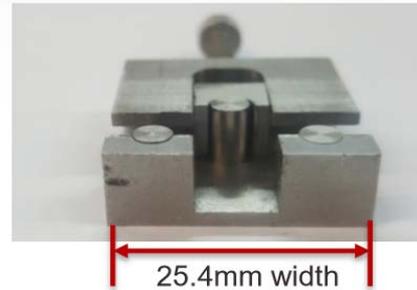
- Using stress-loaded samples to study the effect of stress on corrosion
- Using stress-loaded samples to study the effect of stress on void swelling
- Using pre-irradiated samples to study the effect of irradiation damage on corrosion
- Using simultaneous proton irradiation and corrosion to study the synergistic effects
- Using surface modification to increase corrosion resistance

Key Findings:

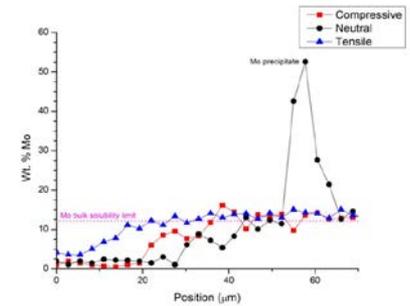
- Deformation induced dislocations can reduce Mo loss towards the surface. Such effects are observed in samples having either tensile stress or compressive stress.
- Ion irradiation can reduce corrosion. Cracking and Mo loss are reduced in the proton-irradiated Hastelloy-N.
- Void swelling is not a concern of Hastelloy-N. No swelling is observed up to 100 dpa.
- Plasma coating can be used to increase the corrosion resistance of stainless steel. Ni layer is deposited on 316L without restriction from sample shapes.

Impact

- The study will help both fundamental studies and materials development to mitigate corrosion issues in MSRs.



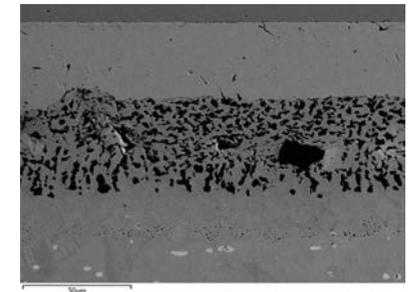
Three-point bending device



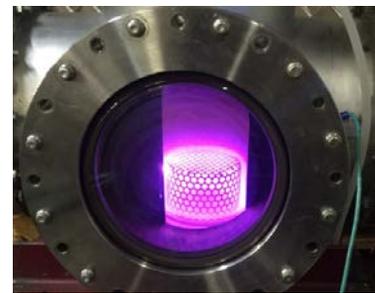
Stress effect on Mo depletion



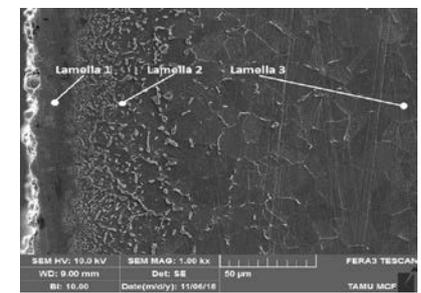
Carbon crucible for corr. test



Corrosion of irradiated Hastelloy N



Plasma coating



Ni coating on a steel

Chemical Technologies



Waste Form Development

- Prepare stable waste form precursors
- Test precursor powders for leach resistance



Sensors Development

- Design and test probes for different operational environments
- Develop data analysis and calibration methods



Salt Characterization

- Develop electrochemical and IR optical methods
- Case study: oxide content quantification



Sensors and Chemical Analysis Workshop

- Assemble experts from industry, national labs and universities to identify state-of-the-art and technology gaps of chemical sensors for MSRs/FHRs

Education and training: development of human capital and expertise

Direct disposal of spent molten salts is not an adequate solution.

- Most halide salts are hygroscopic and oxygen sensitive.
- Radiolysis issues impact long-term halide stability.

A baseline leach was performed on the FLiBe salt

- FLiBe has been tested under the Product Consistency Test (PCT) American Society for Testing Materials (ASTM) Standard C1285
- FLiBe was found to release significant quantities of fluoride ion under the PCT test

Vessel ID	FLiBe Mass (g)	H2O (mL)	pH	F- (ppm)
9	0.7045	7.0	6.31	1131
10	0.6731	7.0	6.24	1024
12	0.7181	7.0	6.45	1161
11	Control	7.5	6.86	2.3



As synthesized FLiBe



Purified FLiBe



FLiBe with TCP (partially reacted)

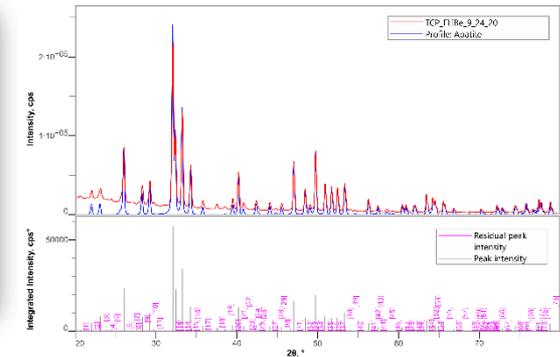


Conversion of Fluoride Salt to Apatite

- The conversion to an apatite required the synthesis of tricalcium phosphate (TCP) were calcium hydrogen phosphate was reacted with calcium carbonate
- Converted FLiBe to fluorapatite by reacting with tricalcium phosphate, confirmed via XRD



Beryllium substituted fluorapatite



Confirmatory x-ray diffraction



Powdered beryllium substituted fluorapatite

Accomplishments:

- Established infrastructure for fluoride and beryllium experimental work
- Prepared fluoride salts for experimental work
- Tested the leach resistance of the salt to establish a baseline
- Determined oxide conversion is not practical
- Converted FLiBe to fluorapatite, confirmed by XRD

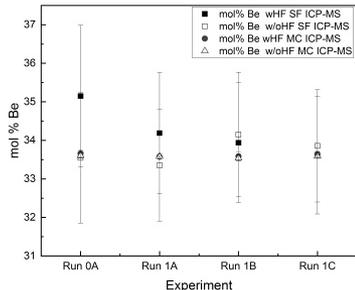
Approach:

- Electrochemical methods
- Complimentary elemental analysis

Elemental analysis

Microwave digestion

ICP-OES, ICP-MS



Square wave voltammetry for oxide quantification

2LiF-BeF₂-Li₂O voltammogram

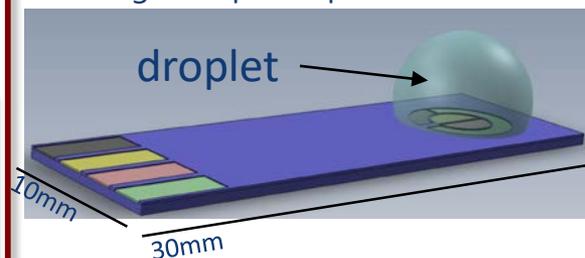


Key takeaways/advantages:

- ➔ Avoid oxygen gas bubbling (clear signal)
- ➔ Fast, online monitoring

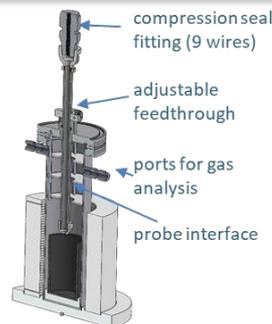
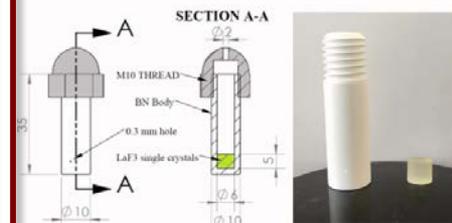
Microfabricated thin film chip sensor

single droplet experimentation



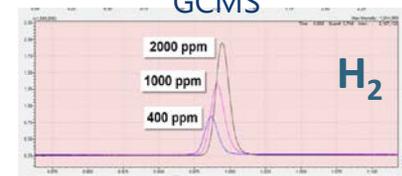
salt.nuc.berkeley.edu

FLiBe thermodynamic reference electrode



Electrochem + gas sparging

GCMS



Highlighted publications & dissemination:

- F. Carotti et al. 2018 Data in Brief 21 1612-1617
- F. Carotti et al. 2019 J. Electrochem. Soc. 166 H835
- A. Consiglio, R.O. Scarlat. *ECS PRiME 2020*. October 4-9, 2020
- H. Williams, R. O. Scarlat. *ECS PRiME 2020*. October 4-9, 2020
- S. Mastromarino, et al. *ACS Meeting*. August 16-20, 2020

VIRTUAL WORKSHOP:

CHEMICAL SENSOR TECHNOLOGIES FOR MSR_s AND FHR_s

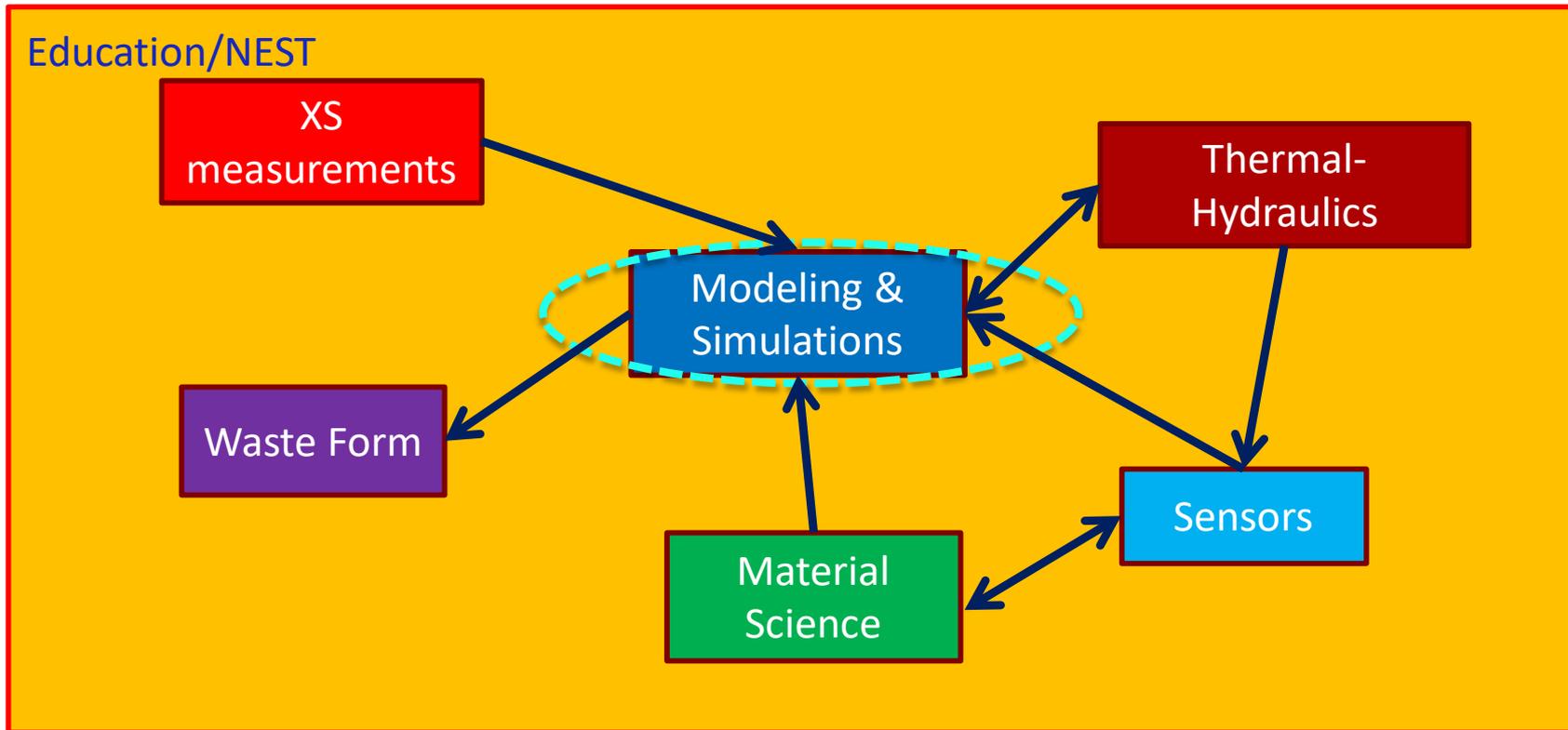
NOVEMBER 12 & 13, 2020
9:00 AM – NOON PT

Purpose: Assemble stakeholders from national laboratories, universities and industry to discuss current state of chemical sensor technologies and identify development needs

Please respond by November 2 by visiting:
salt.nuc.berkeley.edu/chemical-sensors-workshop

Organized under the NuSTEM IRP (nustem.engr.tamu.edu)

Project Components and Integration



1. To contribute to the development of enabling technologies for MSRs
2. To educate young professionals in MSR technologies.

Education Thrust



NEST-Nuclear Education, Skills and Technology Framework



Molten Salt Summer Bootcamp

1-3 July 2019, TU Delft, Netherlands

Capstone Topics

- In-Situ Salt Composition Observation using Optical Techniques (MSR-SCOOT)
- Flow Measurements in MSR: Magnetic, Ultrasound, Simulations
- Nano-MSR Plant
- Ni-Coating for Structural Materials
- Reprocessing for Chloride Fast Reactors
- Solubility for Separations
- Steel Corrosion in Chlorides with Stress & Irradiation
- Helium-Molten Salt HX
- Monitoring of Neutron Flux and Heat Generation



Bootcamp participants and faculty

Modules



Module 1: Multi-physics Modeling

Max Fratoni, Jean Ragusa, and Pablo Rubiolo

Module 2: Thermochemistry: FactSage and Electrochemistry

Ondrej Benes, Anna Smith, and Raluca Scarlat



Module 3: Corrosion and Waste Forms

Adrien Couet, Kumar Sridharan, Raluca Scarlat, Luis Ortega, Sean McDevitt, Anna Smith, and Sylvie Delpech

Module 4: Fuel Cycle

Jiri Krepl and Pavel Tsvetkov



Module 5: Thermal-Hydraulics

Mark Kimber, Stefano Lorenzi, and Antonio Cammi

Education Thrust

NEST-Nuclear Education, Skills and Technology Framework



- Build new generations of skilled and experienced nuclear scientists and engineers (science, safety, waste, NPPs and other relevant technical areas)
- Closer relationship between research organizations and universities, in contact with regulatory bodies or industry needs
- Strengthen capacity at Universities
 - With state-of-the-art knowledge, meeting real world context, with enhanced international relationship
- Attract young generations of professionals

- Natural Resources Canada and U.S. DOE submitted jointly a NEST proposal in 2019.
- Granted in Fall 2019. McMaster U. lead, NuSTEM and SAMOFAR project institutions as co-lead.



Overview Partners Presenters

<https://smrhack.com/>



Small Modular Reactor Virtual Hackathon

9:30 am – 12:00 pm

LECTURES (Stage)

Lead: Adrien Couet, University of Wisconsin

L1-1: Welcome and Assignment of deployment scenarios
John Luxat and Dave Novog, McMaster University

L1-2: International State of Advanced Nuclear Energy Deployment
Jessica Lovering, CMU

L1-3: Micro Reactors vs. SMRs as deployment competition for customers and resources
Pavel V. Tsvetkov, Texas A&M University

1:00 pm – 1:05 pm

WELCOMING REMARKS (Stage)

Rita Baranwal

Assistant Secretary, Department of Energy, Office of Nuclear Energy

1:05 pm – 2:00 pm

TECHNOLOGY ASSESSMENT AND DEVELOPMENT (Stage)

Roundtable of Experts

Paul Wilson, UW-Madison; Sama Bilbao de Leon, OECD-NEA; Steve Bushby, AECL.
Moderator: Adrien Couet, University of Wisconsin

2:00 pm – 3:30 pm

ONLINE CAFE (Hopin Sessions)

Deployment Scenario Teams will each meet on their own

Education Thrust

- **Full courses on MSR:**
 - UW Madison – NE 602 – Molten Salt Technology – Spring 2017 & Fall 2018
 - Lectures available online: <http://nuclearenergy.edublogs.org>
 - UC Berkeley – NE 290B – Special Topics in Nuclear Materials and Chemistry: Molten Salt Chemistry
 - Texas A&M – NUEN 610 MSR Technology module within the nuclear reactor design syllabus – Fall 2018, Fall 2020

New Courses created	Modules/lectures added to existing courses
3	26

Conclusions

- Student outcomes:

NuSTEM Students	
Undergraduate	18
Graduate funded	12
Graduate fellows (NEUP, NRC)	6
Graduate involved	19

- Scholarly productivity:

Literature	
Journal articles	11
Conference proceedings	10
Conference summaries	13

<https://nustem.engr.tamu.edu/>

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NUCLEAR SCIENCE, TECHNOLOGY, AND ENGINEERING FOR
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TEXAS A&M UNIVERSITY

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to develop the technologies and experts
needed for future Molten Salt Reactors**

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