#### A Framework for Multi-physics Modelling, Design Optimization and Uncertainty Quantification of Fast Spectrum Liquid Fuel Molten Salt Reactors

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- This study focuses on Liquid Fuel Molten Salt Reactors (LFMSR)
- LFMSRs do have their fair share of challenges:
  - High temperatures
  - Corrosion
  - Liquid fuel inventory





- This work adopts many aspects from the Euratom Evaluation and Viability of Liquid Fuel Fast Reactor System Project (EVOL) [1]
  - Under EVOL project umbrella, several codes were developed and most of them were based on OpenFOAM C++ code library [2]
  - Similar applications of OpenFOAM can be found in [3-5]



- Optimized core geometry designs are available but lack rigorous studies
- The optimized core geometry (available in literature) is based on one factor i.e. hot spots
- Extensive studies are needed to optimize performance of major systems
- These analyses must consider the multi-physics design impacts on:
  - Plant performance
  - Pump position
  - Placement and sizing of heat exchangers



- Strong coupling between different physics makes the uncertainty analysis more challenging
- Dependencies and interactions between input and non-linear input-output relations add to complexity
- An acceptable framework requires statistical tool(s) that can:
  - Propagate input uncertainties
  - Analyse quantities of interest (QoI) using appropriate statistical tools
  - DAKOTA is utilized in this work



## **Objectives**

- Identify and model the multi-physics phenomena that impose potential challenges:
  - Structural material temperature limits
- Develop high-fidelity CFD models of LFMSRs
- Perform uncertainty propagation, sensitivity analysis, and design optimization studies of the LFMSR system

• General framework for multi-physics UQ



- This work uses GeN-Foam (General Nuclear Field Operation And Manipulation) for multi-physics modeling [7]
  - Based on Open-source Field Operation And Manipulation (OpenFOAM) C++ library
  - Capable of modeling both light water reactors and liquid fueled systems
  - Compatible with structured or unstructured meshes to model a geometry





- Thermal-hydraulics sub-solver uses modified Reynolds-Averaged Navier-Stokes (RANS) equations
- The solver can evaluate both RANS and porous medium RANS equations
  - This work used the standard k-epsilon turbulence model with porous media approximation
  - Heat exchanger and pump are modeled as porous regions
- Main equations solved through a merged PISO-SIMPLE (PIMPLE) pressure-based algorithm
- More information can be found in [7]

### **Methods**

• Neutronics sub-solver is based on multigroup diffusion equation

$$\frac{1}{v_g}\frac{\partial \varphi_g}{\partial t} = \nabla \cdot D_g \nabla \varphi_g - \Sigma_{r_g} \varphi_g + \sum_{g' \neq g}^G \Sigma_{g' \rightarrow g} \varphi_{g'} + \chi_{p,g} \big(1 - \beta_{eff,t}\big) \sum_{g'=1}^G \nu \Sigma_{f,g'} \varphi_{g'} + \sum_k^{G_d} \chi_{d,g}^k \lambda_k C_k$$

• The delayed neutrons precursors equation is given by:

$$\frac{\partial C_{k}}{\partial t} + \nabla \cdot (u_{D}C_{k}) + \nabla \underline{\cdot} \frac{\nu_{t}}{Sc_{t}} \nabla C_{k} = \frac{\beta_{eff,k} \sum_{j} \nu \Sigma_{f,j} \varphi_{j}}{k_{eff}} - \lambda_{k}C_{k}$$

## **Methods**

- The LFMSR concept is a 3000 MW<sub>th</sub> reactor:
  - Fast-spectrum breeder reactor with a large negative power coefficient
  - The liquid salt serves as both fuel and coolant
  - Reduced reprocessing requirements and better reactor breeding ratios are possible with this type of reactor [6]
  - All model inputs are adopted and derived from this design



#### Adopted from [1]

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- Gen-Foam thermal-hydraulic conditions
  - Fuel salt: 1 · PuCl<sub>3</sub> 8 · UCl<sub>3</sub> 10 · NaCl
  - Inlet salt velocity was 1 m/s, inlet temperature of 650 K
  - Model was evaluated at steady conditions

PARAMETER	VALUE	UNITS
Density	4200	kg/m³
Specific Heat Capacity	950	J/kg-K
Dynamic Viscosity	0.00217	Pa-s
Thermal Expansion Coefficient	0.000464	1/K
Thermal Conductivity	0.7	W/m-K



- Gen-Foam neutronics conditions
  - Vacuum boundaries were set at the walls
  - Reflective boundary set along the symmetry line, inlet, and outlet
  - Serpent 2.1.32 was used to generate the parameterized cross sections
  - MATLAB script converts cross sections into a format readable by GeN-Foam
  - GeN-Foam uses an interpolation method to calculate the cross sections between different physical states
  - Model was evaluated in steady conditions





- Multi-physics UQ framework was applied to temperature limits of LFMSR primary loop components
  - Proposed materials are Stainless Steel (SS) 316L and Hastelloy-N

PARAMETER	VALUE	UNITS
Salt Melting Temperature	739	K
Salt Boiling Temperature	1673	K
Maximum Hastelloy N Operational Temperature	990	K
Maximum SS 316L Operational Temperature	1658	K

- Two power levels (25, 50 MW<sub>th</sub>), three heat transfer coefficients (1, 2.5, 5 kW/m<sup>2</sup>-K) and three pump heads (5, 10, 20 kN/m) were evaluated with a 2D GeN-Foam model
- Case indices were numbered according to combination of input parameters (see table to right)

INDEX	POWER (MW)	HTC (kW/m²-K)	PUMP HEAD (kN/m)
1	25	1	5
2	25	1	10
3	25	1	20
4	25	2.5	5
5	25	2.5	10
6	25	2.5	20
7	25	5	5
8	25	5	10
9	25	5	20
10	50	5	5
11	50	5	20
12	50	2.5	5
13	50	2.5	10
14	50	2.5	20
15	50	1	5
16	50	1	10
17	50	1	20

- DAKOTA is the Design and Analysis toolKit for Optimization and Terascale Applications [8]
- Performs statistical analysis on code output and subsequently adjusts code input
- Supports several sampling techniques such as Monte Carlo (MC) sampling, Latin Hypercube Sampling (LHS), and Grid Sampling



- GeN-Foam was coupled to DAKOTA and the inputs were varied between 2-20% (see table)
- All variables were given a normal distribution

PARAMETER	VARIATION
Density	2%
Specific Heat Capacity	20%
Dynamic Viscosity	10%
Thermal Expansion Coefficient	15%
Heat Transfer Coefficient	20%
Pump Head	20%



## **Results and Discussion**

- Indices 2, 3, 5, 6, 9, 10, 13, and 14 fall within the set limits for SS 316L
- The SS 316L material has a much higher operating temperature limit and allows for more flexibility



## **Results and Discussion**

- Only indices 5 and 9 fall within the set limits for Hastelloy-N
- Hastelloy-N has a lower maximum operating temperature



### **Results and Discussion**

- Only two conditions (indices) fell within operating temperature limits for both SS 316L and Hastelloy-N
  - 25 MW<sub>th</sub>, 2.5 kW/m<sup>2</sup>-K, 10 kN/m
  - 25 MW<sub>th</sub>, 5 kW/m<sup>2</sup>-K, 20 kN/m
- Other physical effects may need investigation
  - Corrosion
  - Thermal fatigue / striping
  - Radiation damage

## Conclusions

- When considering only the average coolant outlet temperature, SS 316L has more flexibility than Hastelloy-N
- Methodology can be extended to any other design criteria or input
  - Other effects can be investigated with the same methods
- Successful coupling of high-fidelity physics with UQ tools can provide a robust method for reactor design analysis

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