Roadmap to Establish an Integrated TPBAR Performance Model

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briefly describe observations, transportation pathways and implications within the current technology

describe the approach and goal

- Methodically build a collection of mechanistic models that are effectively integrated

- Extrapolation of TPBAR performance and behavior to new conditions and designs

provide some examples of progress made since Oct 2016

discuss path towards implementation over the next 9 months
BAR Observations and Implications

2004, during Cycle 6, it was determined that TPBAR tritium permeation was higher than predicted by performance models
- Predicted ≈ 0.5 Ci/TPBAR/cycle
- Actual ≈ 4 Ci/TPBAR/cycle

4 Ci/TPBAR/cycle represents only about 0.04% of the tritium produced.

The mechanisms responsible for differences between predictions and observations are not well characterized or understood.

Increasing the number of TPBARs per cycle increases tritium permeation.
BART Design Transport Pathways

Cycle 6 demonstrated original vision was inadequate. IE and ex-reactor testing led to revised vision that drove Mark 9.2 design. Subsequent TPBAR experiments suggested that Mark 9.2 model does not fully explain performance:

- Pellet speciation and burnup dependencies
- Carbon transport and deposition
- Tritium transport and distribution

Cycle 13 and TMIST-3 provide unique opportunity to focus on pellets.

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Tritium Transport within TPBAR

Original Vision

- Pellets
  - \( \text{T}_2 \text{O} \)
- Liners
  - \( \text{T}_2 \)
- Getter
  - \( \text{T}_2 \)
- Cladding
  - \( \text{T}_2 \)
- Coolant

Mark 9.2 Vision

- Pellets
  - \( \text{T}_2 \text{O} \)
- Liners
  - \( \text{T}_2 \)
- Getter
  - \( \text{T}_2 \)
- End Plugs/Cladding
  - \( \text{T}_2 \)
- Coolant
Current Pellet Model Approach

- **Neutronics**
  - Serpent2
  - VERA

- **Pellet Retention**
  - OpenFOAM
  - MISTRAL
    - (fusion reactors tritium breeder modeling)

- **Microstructural Evolution**
  - Phase Field

- **Thermal Conductivity**
  - Phonon-transport

- **Gas Diffusion**
  - Phase Field

- **Integration**
  - Python

**H3FR**

**MACHINE LEARNING**

**MD Simulations**

**Tritium Science**
Investigating the use of MISTRAL

- Tritium transport model used to design and evaluate the performance of lithium breeder blankets for fusion reactors (ITER)
- The model includes the following physics:
  - Production of tritium within the grains (ambipolar diffusion)
  - Migration of tritium to the grain boundaries
  - Gas motion along grain boundaries to the network of interconnected pores
  - Adsorption/desorption and surface reactions
  - Porous diffusion
- MISTRAL has been validated against in-situ tritium extraction experiments (LISA1, MOZART)
- An implementation of MISTRAL and ambipolar diffusion models is being developed in Matlab as prototype
- Will move to FOAM when complete with multi-physics integration

Multi-Ionic diffusion model containing ambipolar diffusion model. Model has been benchmarked against numerical solutions for a glass couple. H+ concentration in the pellet for debugging.
**Phase Field Diffusion Model**

Develop model on larger scale to study dpa rates and defect mobility on defect accumulation under ion irradiation and neutron radiation. Compare with analytical and experimental results. Consider irradiation-enhanced phase transition (LiAlO$_2$ → Al$_5$O$_8$).

- Example of phase transition and microstructure evolution in irradiated polycrystalline LiAlO$_2$ for given concentrations of Li, O, and vacancies. Phase field model for Al$_5$O$_8$ and void evolution.
SEM imaging of irradiated LiAlO2 pellet from C11. The images show the entire outer pellet edge and progressively higher magnification showing the nature of transmutation effects in the material with the formation of Li-depleted phases, voids, and opening of grain boundaries.
Model pellet thermal conductivity degradation using phonon transport models
OpenMOC is being investigated for this purpose
- Readily solve fixed source problems
- Input files written in Python
- Multi-group transport code (frequency dependent phonon transport)
- Combinatorial geometry capability
- Lower computational cost
Develop feature for incident angular flux boundary conditions – necessary for phonon transport calculations
Implement a feature to read-in nuclear data files
Focus on obtaining location / time-dependent irradiation history of TPBAR components to assist with PIE and data analysis

- Full core depletion with coupled neutronics / thermal hydraulics modeling
- Pin-by-pin resolution, either using transport or SPn methods
- Capability to define customized cross-section sets for TPBARs or other applications
- Capability to perform adjoint calculations to treat problems as secondary sources or tritium production optimization
- Advanced edits and visualization capabilities to enhance understanding of tritium production in core
- Provide time and space-dependent information on tritium production or other isotopes of interest
- Microscopic depletion is used in the model, allowing for tracking of single isotopes in the core and throughout the cycle

A number of sample problems have been executed with VERA 4 and VERA 3.6

- Includes 2-D lattice physics problems, with and w/o TPBARs and full size 3-D assemblies
- Model is responding correctly
FR – H³ Framework

- Self-contained code base that utilizes active TROD input structure
- NN surrogate model
  - Given inputs/outputs, develop a model to describe the behaviors with 40k simulations
  - TROD is quick and easy; not all modeling tools will be
- Preliminary assessment is underway
  - Progress made on development and validation of code base
  - Interested in how variables interact, not the “right” answer
- Utilizing short cycle, rod average case (469 EFPD)
  - Training conducted with a 4 layer MLP
    - 320, 240, 120, 80 nodes per layer
    - 26 inputs
    - 64 outputs
  - RELU activation layers