



Blanket Modeling with Tritium Accountancy using MELCOR-Fusion

June 2024

Changing the World's Energy Future

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**Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517**

June 5, 2024

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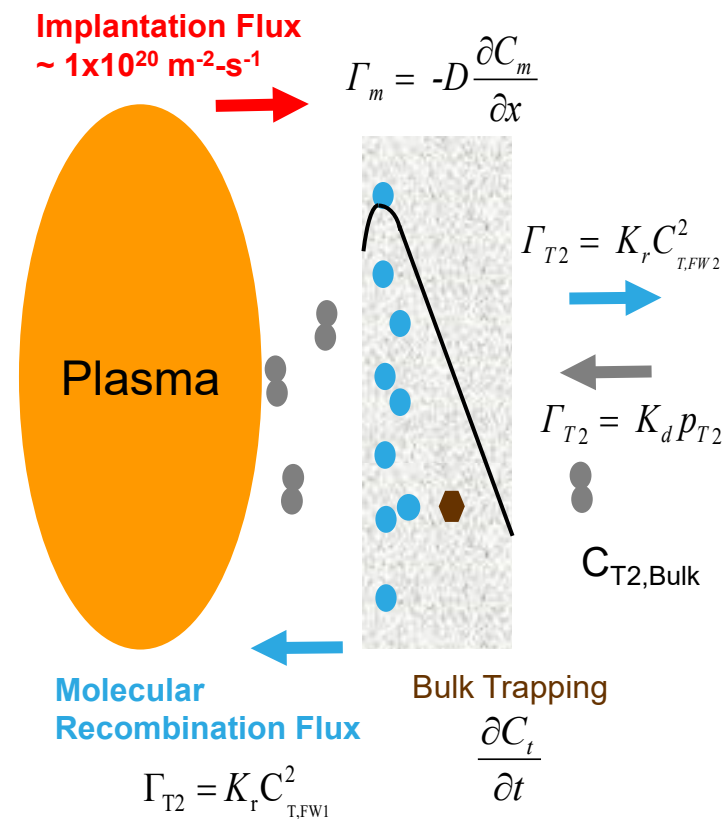
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Fusion Safety Overview

- DOE Fusion Safety Standard collects existing regulatory limits and standards, and provides guidance on how to meet these in a magnetic fusion reactor
 - Identifies two additional requirements for fusion, on dose and waste:
 - < 10 mrem/yr dose to public from normal operations
 - The need for an off-site evacuation plan shall be avoided
 - Implies < 1 rem dose at site boundary in accident scenario
 - Wastes, especially high-level radioactive wastes, shall be minimized
- Safety and tritium analyses are conducted with MELCOR/TMAP to understand radionuclide distribution and transport during normal and accident scenarios, from the point of generation to the site boundary

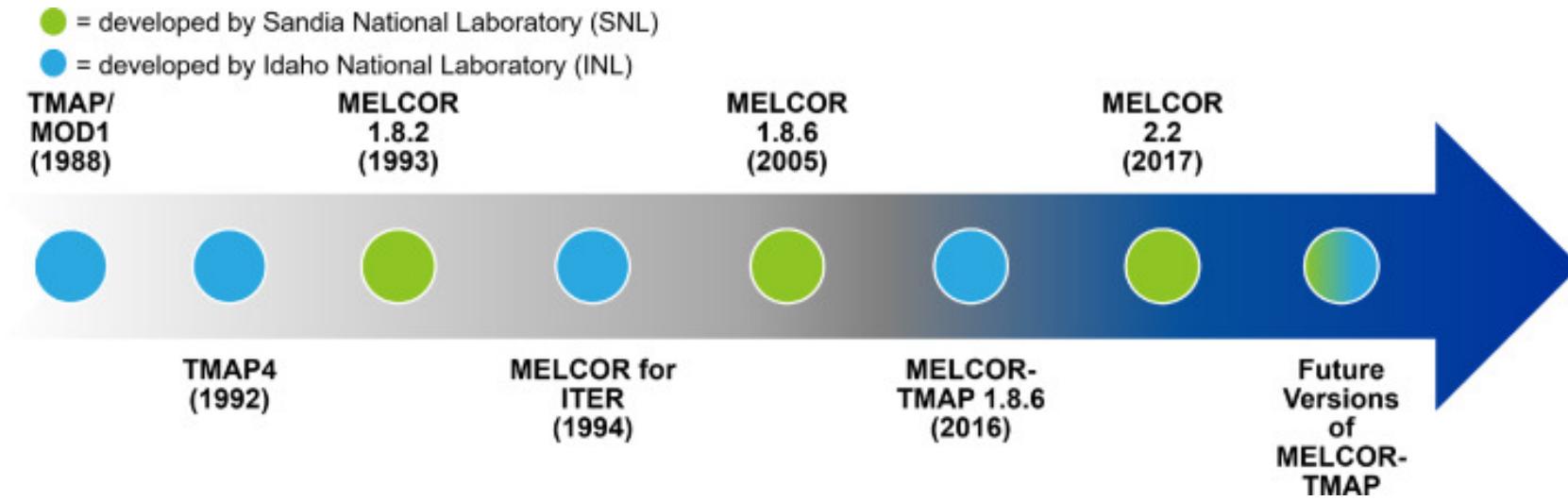
TMAP

- TMAP (Tritium Migration and Permeation) is a code that models diffusion and trapping of hydrogen isotopes in structures and flow through connected enclosures
- It was developed at INL in the late 1980s as a tool for safety analysis of systems involving tritium
 - TMAP/MOD1 released (limited distribution) in 1988
 - Verified and Validated TMAP4 released in 1992
 - Long available via (now defunct) Energy Science and Technology Software Center (ESTSC) and (still) widely used
 - Followed by TMAP5 (not released), and
 - TMAP2000 (not verified and validated)
 - Most recent release is TMAP7 in ~2004
 - Addressed several issues with TMAP4 and introduced some new features
 - Multiple traps
 - Radioactive decay
 - Extended problem size



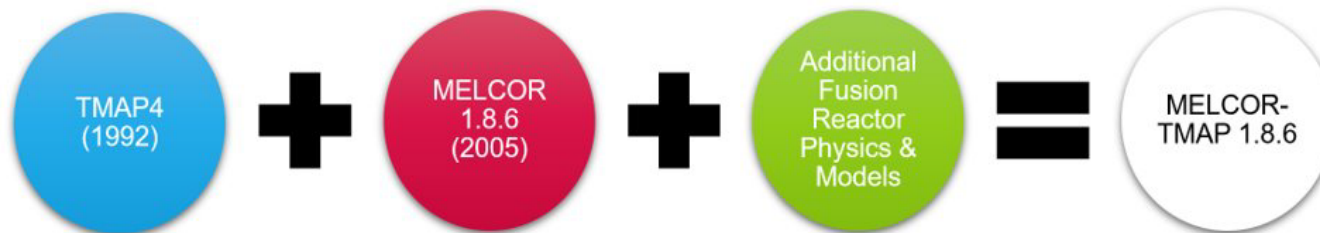
History of MELCOR-Fusion

- Forked from MELCOR 1.8.2 for the development of ITER
 - EOS modifications to allow for water freezing and ice layer formation
 - Aerosol transport modifications to properly account for gas mixtures, turbulent and inertial deposition mechanisms
 - Radiation heat transfer in enclosures
 - Tritium transport (as HTO)
- MELCOR-ITER 1.8.2 has been “pedigreed” and used in ITER NSSR 1&2, GSSR, RPrS and is still used today



MELCOR for Fusion

- Additional modifications to later versions of MELCOR (1.8.5/1.8.6) were made to model advanced fusion reactor concepts, including:
 - RELAP/ATHENA fluid properties including Li, PbLi, Sn, SnLi, FLiBe, real EOS for hydrogen, helium
 - Lithium pool fire models similar to LITFIRE
 - Aerosol resuspension models
 - Different multiphase fluids in different loops
 - Full integration of tritium transport models from TMAP
- All these models recently integrated into a single code based on MELCOR 1.8.6, which we call MELCOR/TMAP
- Work to incorporate MELCOR-Fusion models into MELCOR 2.2 is ongoing



- Tritium migration
- Trapping, diffusion, solubility
- Multiple species tracking

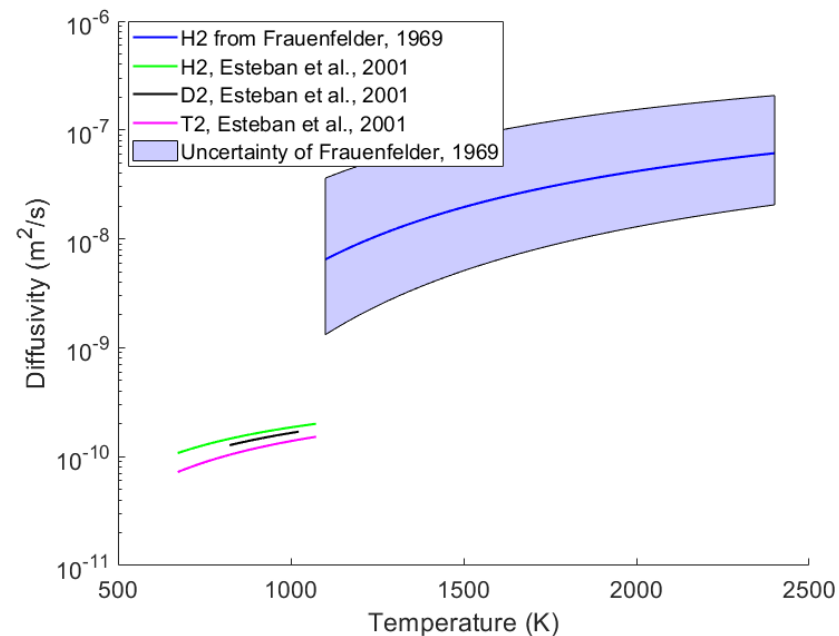
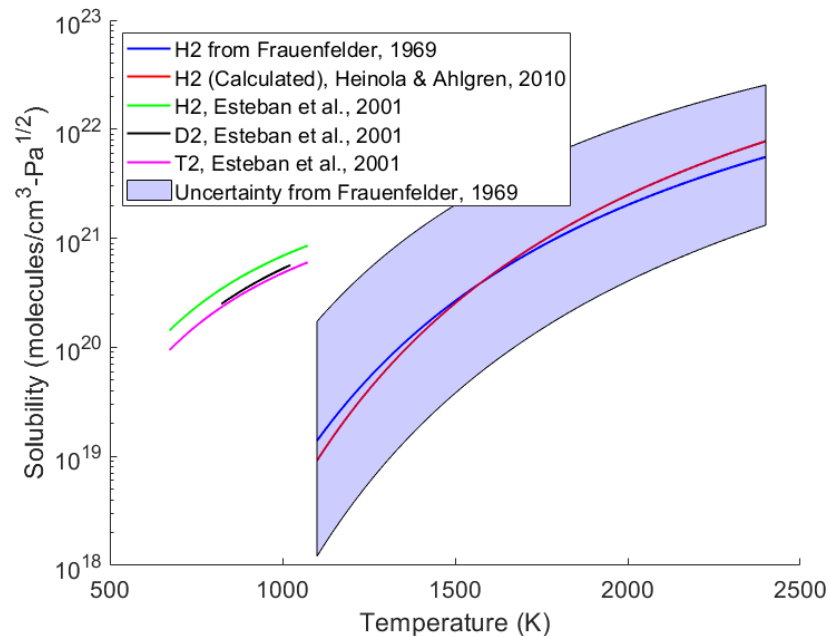
- Heat transfer
- Thermal hydraulics
- Vapor & aerosol tracking
- Reactor accidents

- HTO modeling
- Lithium fire accidents
- Multiple working fluids

- Fully integrated capabilities
- Steady-state & transient analysis including accident scenario simulations

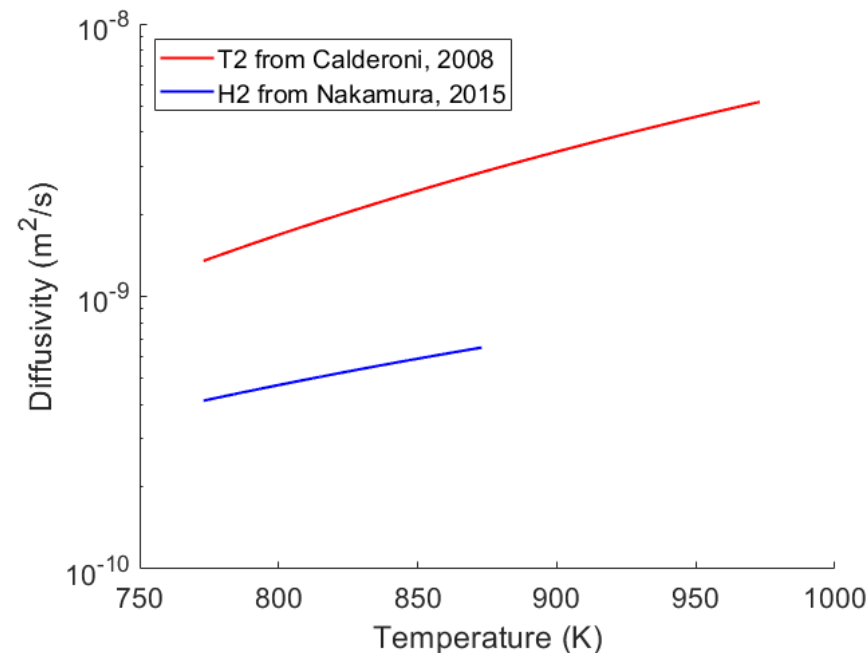
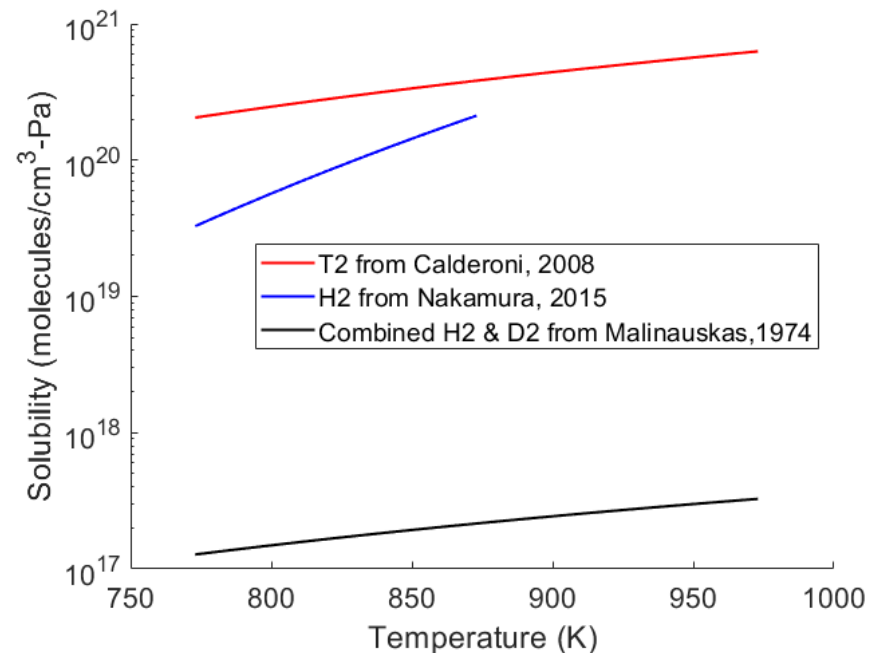
Tritium transport through tungsten is uncertain

- Estimates of solubility of tritium in tungsten vary by three orders of magnitude
- Estimates of tritium diffusivity in tungsten vary by four orders of magnitude
- We take Frauenfelder's 1969 material properties for our base case



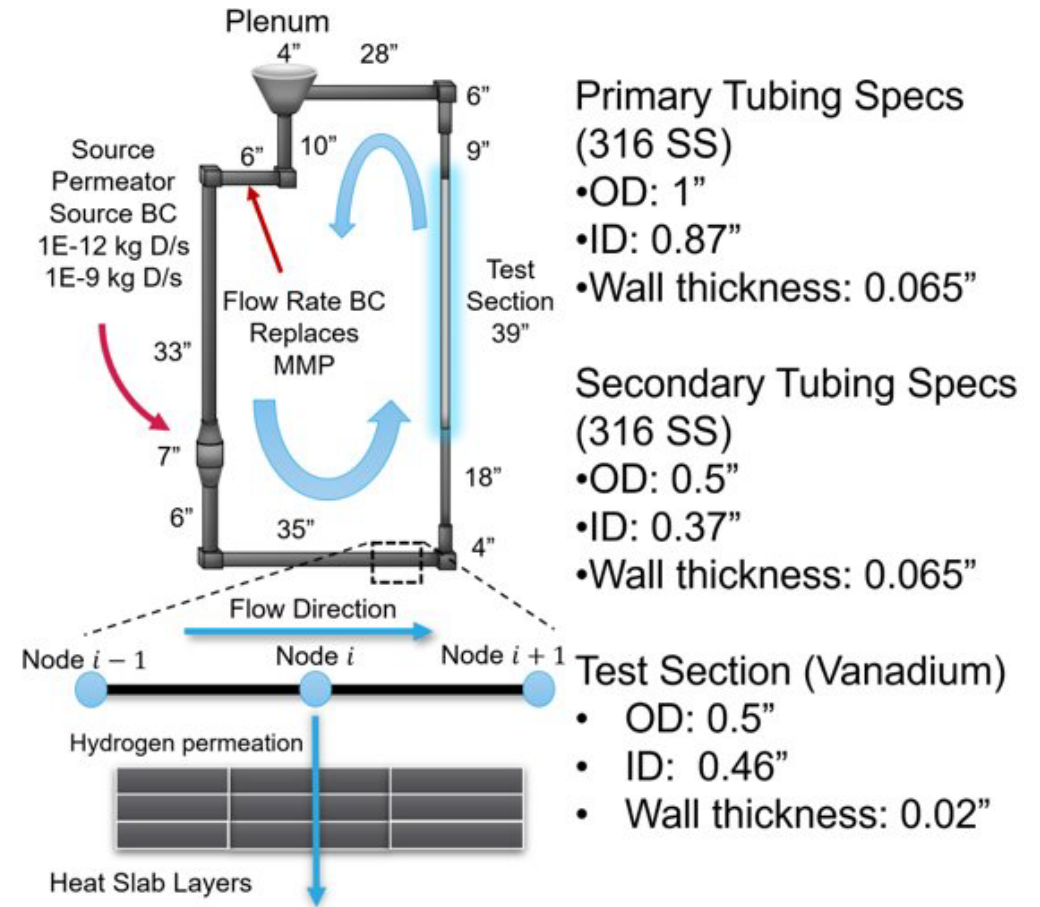
Experimental work on tritium transport in FLiBe

- There is a lack of experimental data on the solubility and diffusivity of tritium in FLiBe
- Existing data shows several orders of magnitude uncertainty
- We will take Calderoni's 2008 work for our base case



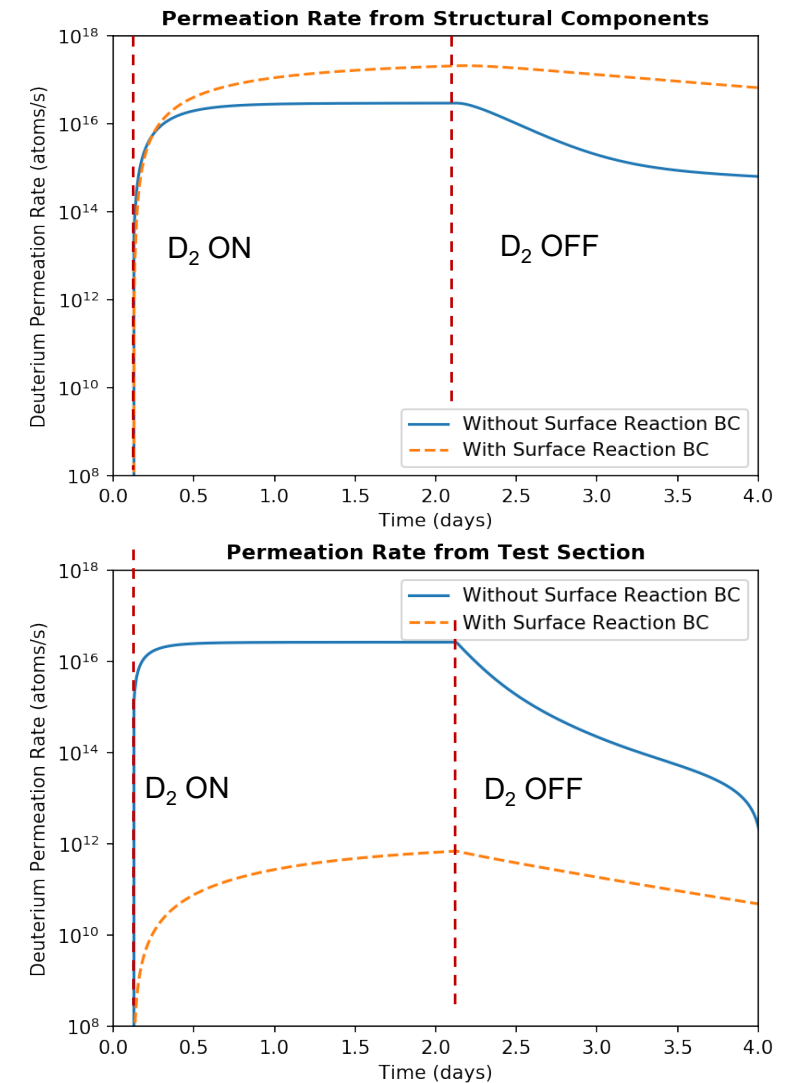
TEX Model in MELCOR-TMAP

- Control volumes (CVH) used to represent pipes, plenum, source permeator, test section, vacuum, and surrounding volumes
- Flow paths (FL) track advection of moving fluid (PbLi) and hydrogen species between control volumes
- Heat structures (HS) used to simulate solid walls and interfaces through which hydrogen permeates



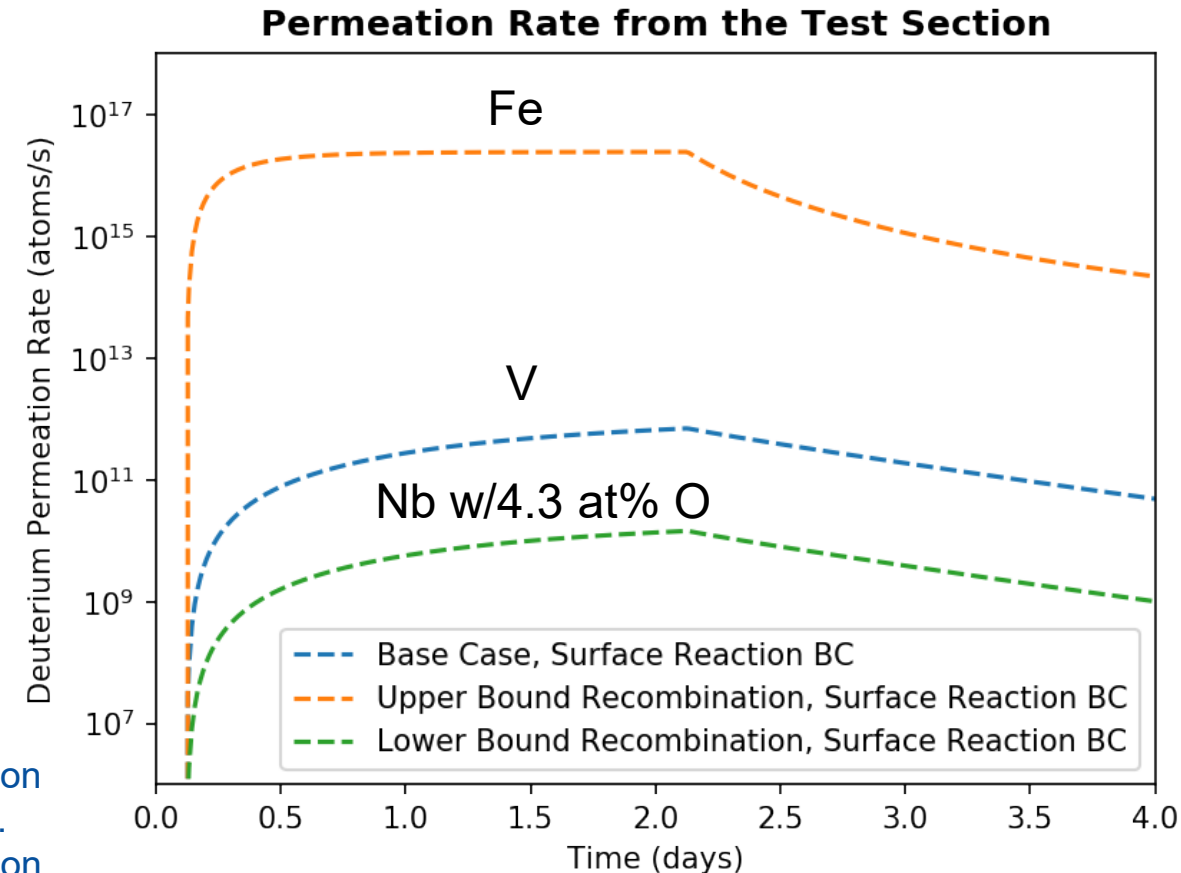
MELCOR-TMAP Simulations

- Deuterium source:
 - Source boundary condition: $3e+17$ atom/s source term, 48 hours ON and 48 hours OFF
- Permeation rates and transient behavior depend on boundary conditions applied (solution law vs. surface reaction rates)
- Surface-reaction BC accounts for:
 - Recombination of deuterium on the outside of test section and piping
 - Solution law BC at the PbLi-tube interface (i.e., Sieverts' law)
 - Dissociation from atmosphere back into the tubing + PbLi (unlikely)
- Simulation results demonstrate permeation rate from test section impacted heavily by surface reaction rate BC; confirms the outer test section material must be carefully chosen for suitable material properties (i.e., solubility and recombination)



Sensitivity to Permeator Recombination

- Permeator recombination modified:
 - Upper bound¹: Fe recombination
 $= 5.9e-27 \cdot \exp(-0.20/kT) \text{ m}^4 \cdot \text{molecule}/(\text{s} \cdot \text{atom}^2)$
 - Nominal case²: V recombination
 $= 7.6e-25 \cdot \exp(-1.32/kT) \text{ m}^4 \cdot \text{molecule}/(\text{s} \cdot \text{atom}^2)$
 - Lower bound³: Nb with 4.3 at% O
 $= 2.6e-30 \cdot \exp(-0.81/kT) \text{ m}^4 \cdot \text{molecule}/(\text{s} \cdot \text{atom}^2)$
- Results demonstrate permeation rate is highly sensitive to recombination of permeator material, ranging in ~6 orders of magnitude from lower to upper bounds



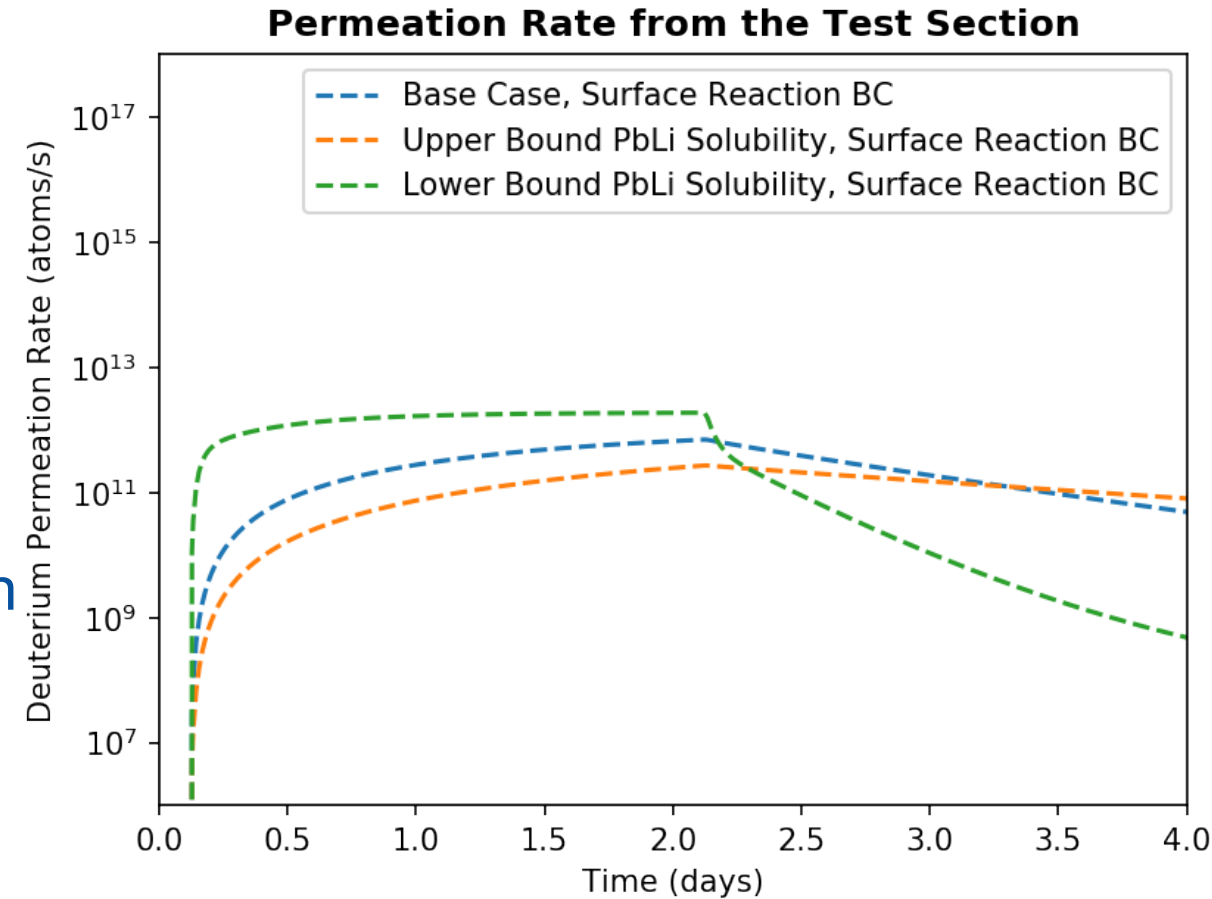
¹F. Waelbroeck, I. Ali-Khan, K.J. Dietz, P. Wienhold. 1979. "Hydrogen solubilisation into and permeation through wall materials." J. Nucl. Mat. 85-86 Part 1: 345-349.

²T. Fuerst, P.W. Humrickhouse, C.N. Taylor, M. Shimada. 2021. "Surface effects on deuterium permeation through vanadium membranes." J. Membrane Sci. 620:118949

³R. Hayakawa, A. Busnyuk, Y. Hatano, A. Livshits, K. Watanabe. 2003. "Relation between Recombination Rate Constant of Deuterium at Niobium Surface and Oxygen Concentration in Bulk." Physica Scripta 113.

Sensitivity to PbLi Solubility

- PbLi solubility modified:
 - Upper bound¹
 $= 3.6\text{e}+22 \text{ atoms}/(\text{m}^3\cdot\text{Pa}^{1/2})$
 - Nominal case²
 $= 1.4\text{e}+23 \cdot \exp(-0.13/kT) \text{ atoms}/(\text{m}^3\cdot\text{Pa}^{1/2})$
 - Lower bound³
 $= 7.7\text{e}+20 \cdot \exp(-0.01/kT) \text{ atoms}/(\text{m}^3\cdot\text{Pa}^{1/2})$
- Results show solubility affects rate of change in permeation rate, but doesn't greatly affect the SS permeation value



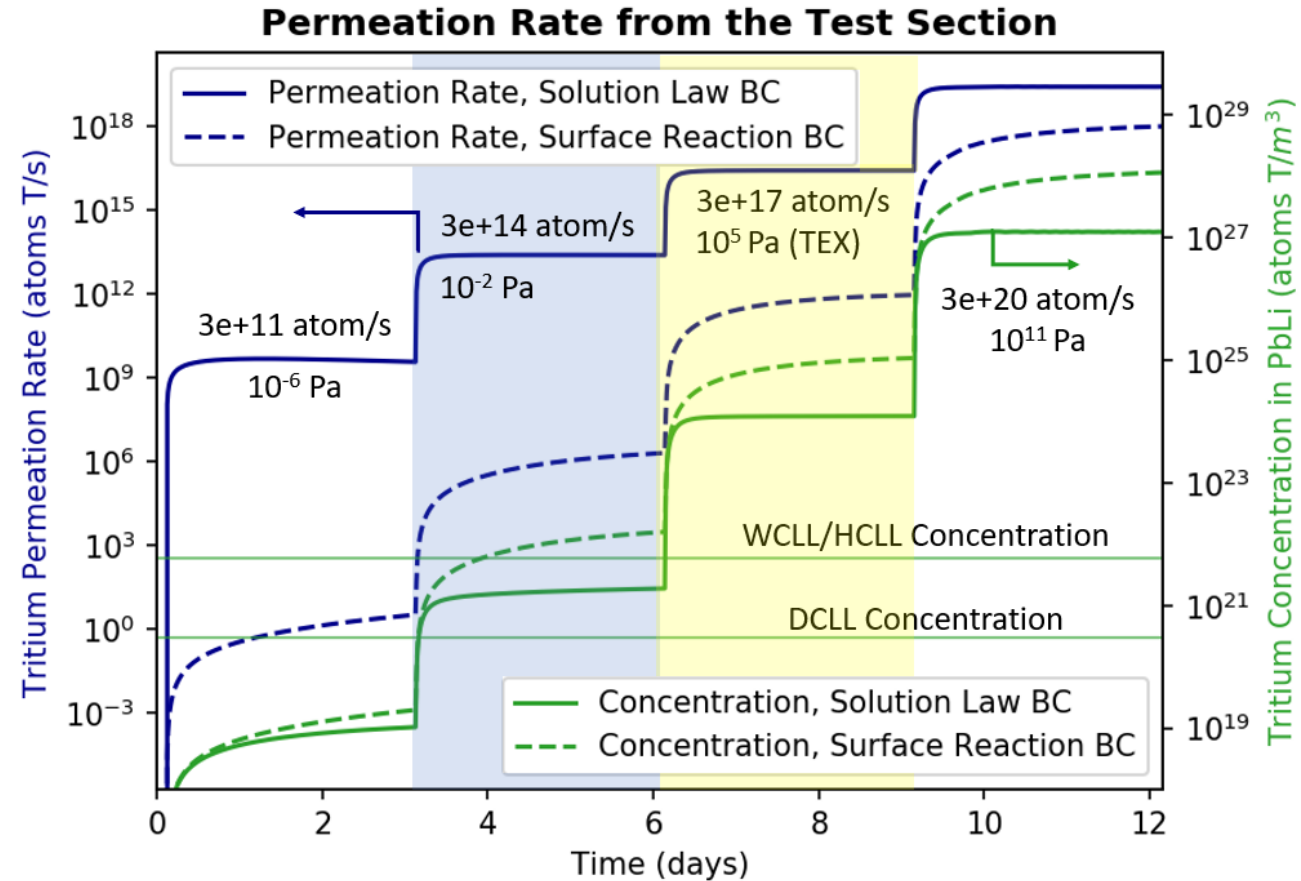
¹H. Katsuta et al. 1985. "Hydrogen Solubility in Liquid Li17-Pb93." J. Nucl. Mater. 133-134: 167-170.

²A. Aiello, Ciampichetti A., and Benamati G. 2006. "Determination of hydrogen solubility in lead lithium using sole device." Fusion Eng. Des. 81, no. 1: 639-644

³F. Reiter. 1991. "Solubility and diffusivity of hydrogen isotopes in liquid Pb-17Li." Fusion Eng. Des. 14: 207-211.

Sensitivity to Source Rate

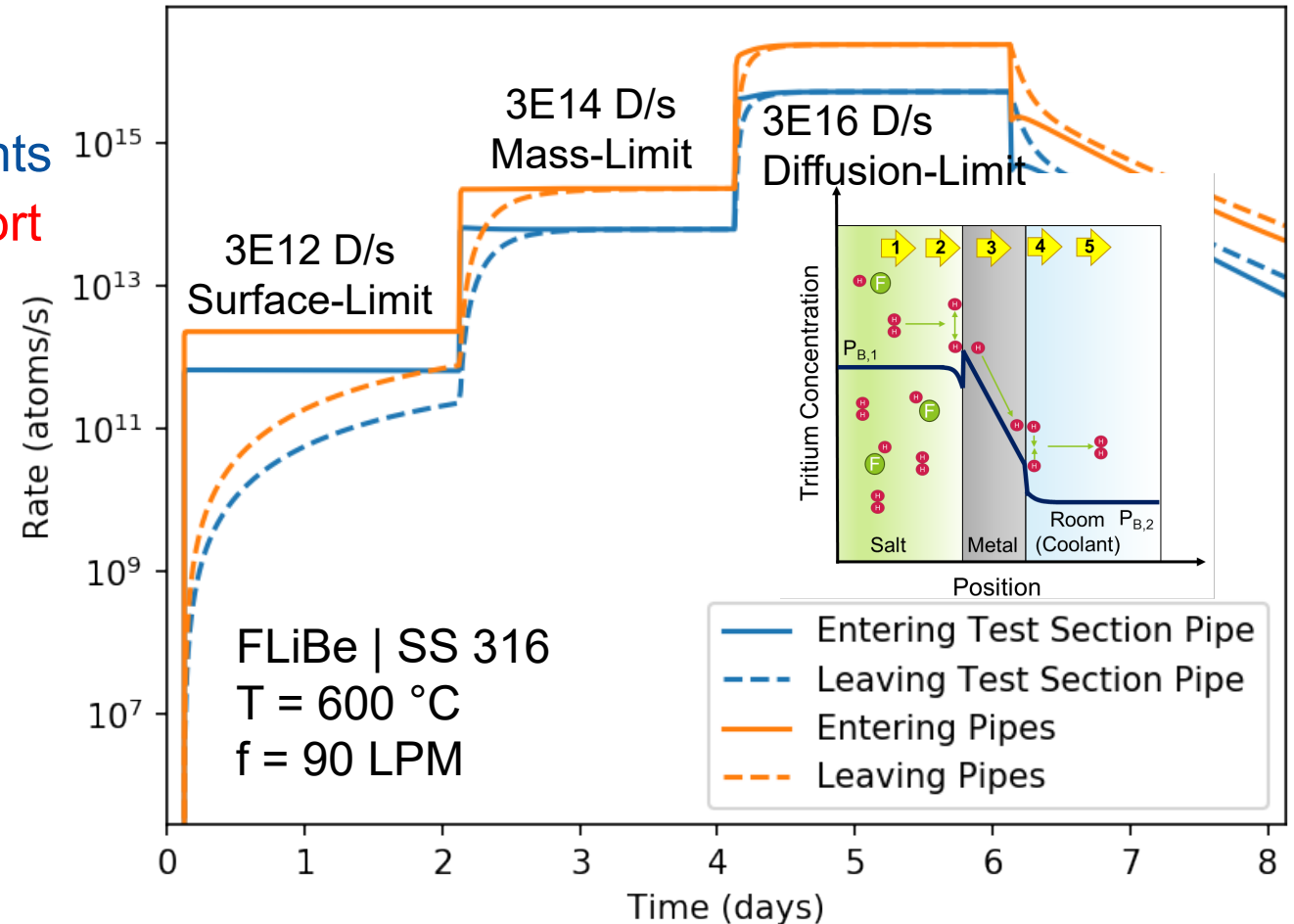
- Source rate was ramped up between $3e+11$ to $3e+20$ atom/s for 3 days at a time
- Simulations show permeation rate from test section are highly sensitive to source rates
 - Surface reaction rates matter less (converge) as the deuterium concentration in PbLi increases (departing from surface-limited regime)



Experimental Campaigns

- Variables:
 - **Flow Rate:** Salt Mass Transfer Coefficients
 - **Source Term:** Permeation Mass Transport
 - **Temperature:** Arrhenius Dependence
- Example Procedure:
 1. Loop heat up
 2. Pump priming
 3. Start hydrogen injection
 4. Stop hydrogen injection
 5. Stop pump
 6. Cool down

Modeled with Melcor-TMAP [1]



Gas-phase H/D/T permeation systems at INL

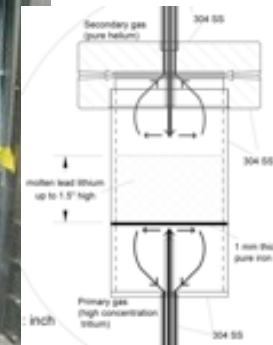
Static Gas Absorption Permeation (SGAP)

- $10^0 < p_{Q_2} [\text{Pa}] < 10^5$ (where Q=H or D)
- Absorption: up to 950 °C (1223K)
- Permeation: up to 900 °C (1173K)
- Vertically standing furnace capable of testing
 - Liquid (e.g. PbLi)
 - Disc from 6 mm to 25 mm OD
- Moderately radioactive materials handling
 - Dose rate limit $< 1 \text{ mSr/hr @ 30 cm}$



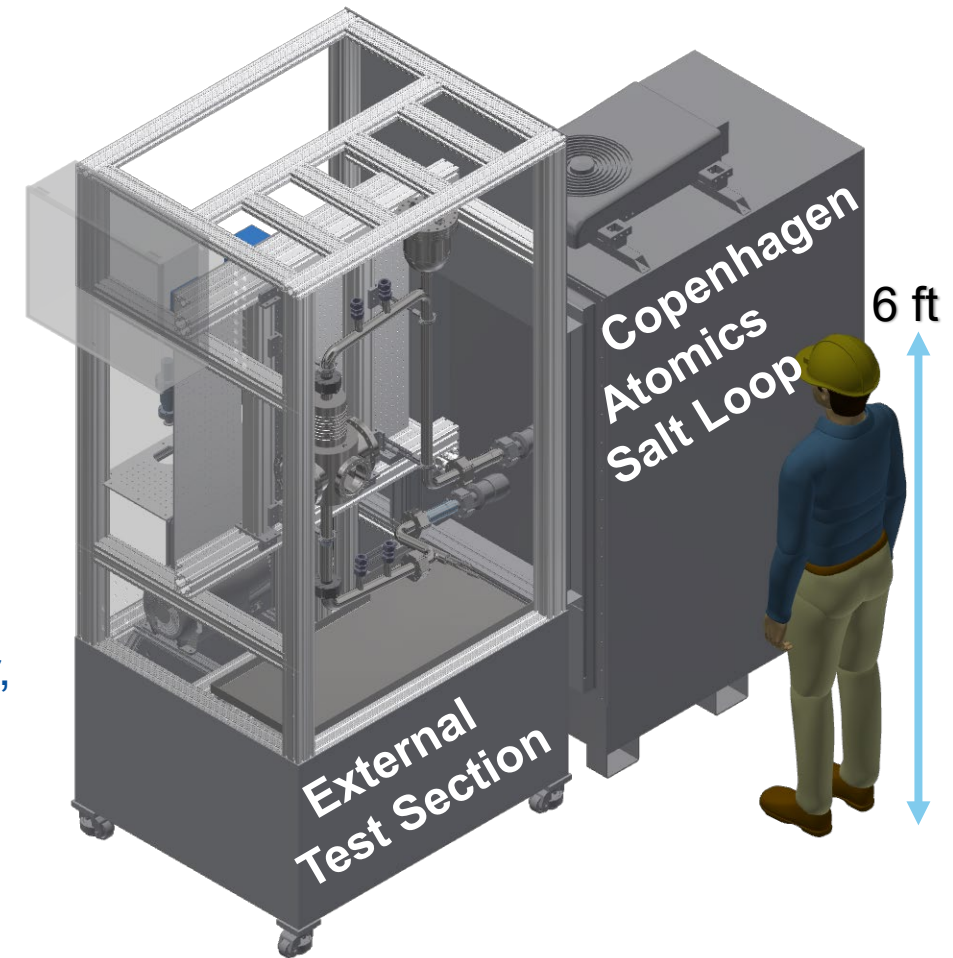
Tritium Gas Absorption Permeation (TGAP)

- Low tritium partial pressure = extreme sensitivity
 - $10^{-12} < p_{T_2} [\text{Pa}] < 10^0$
 - Tritium limit: 25 Ci per campaign
- Absorption & Permeation: up to 700 °C (973K)
- Vertically standing furnace capable of testing
 - Liquid (e.g. PbLi)
 - Disc specimen from 6 mm to 25 mm OD
- Moderately radioactive materials handling
 - Dose rate limit $< 1 \text{ mSr/hr @ 30 cm}$



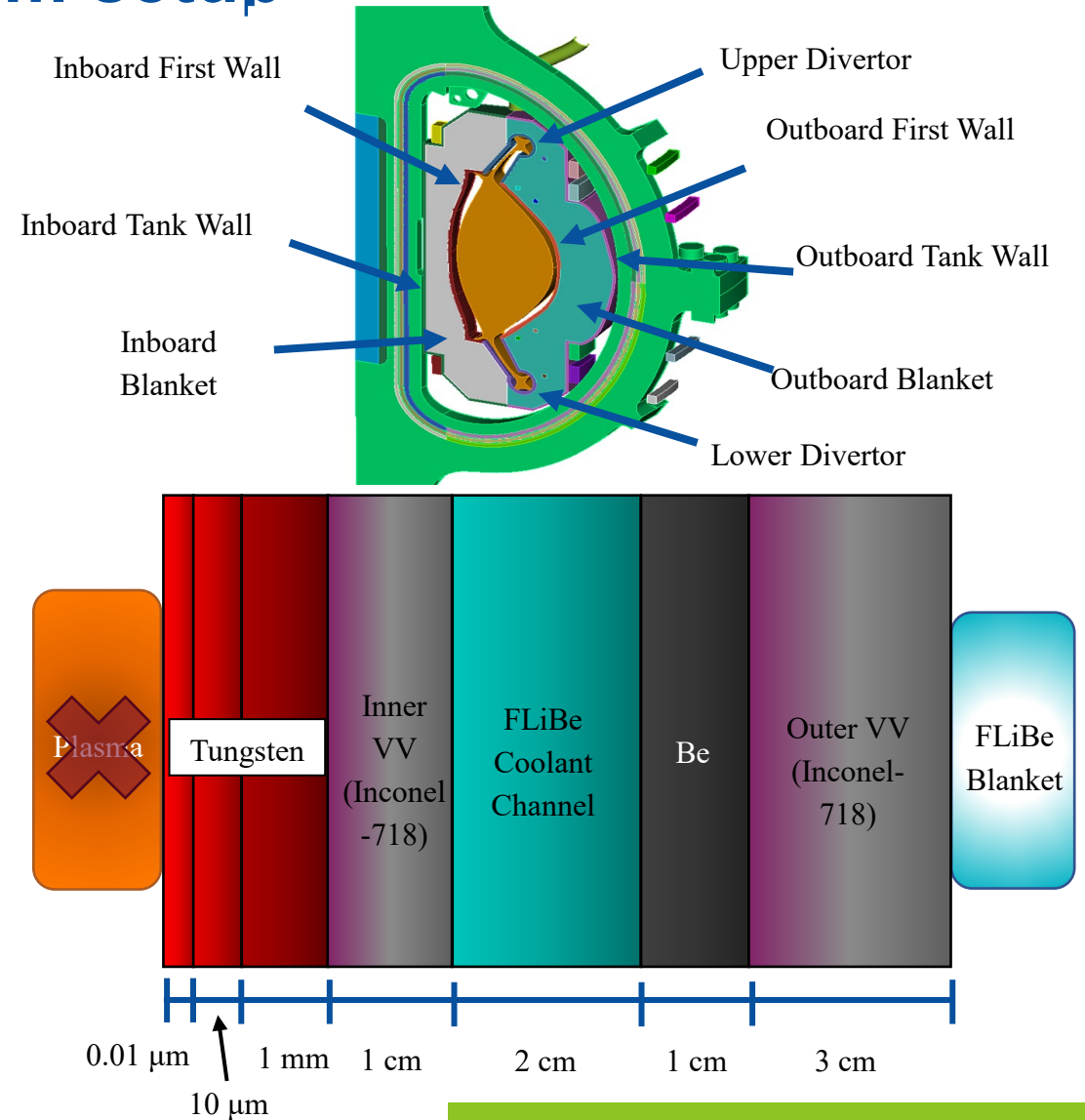
Molten Salt Tritium Transport Experiment

- *MSTTE is a semi-integral tritium transport experiment for flowing fluoride salt systems.*
- Location: Safety and Tritium Applied Research facility at Idaho National Laboratory
- **Objectives:**
 - (1) Safety code validation data.
 - (2) Test stand for tritium control technology.
- **Major Equipment:**
 - **Copenhagen Atomics Salt Loop:** salt tank, pump, flow meter, instrumentation and control
 - **External Test Section:** hydrogen injection, permeation, plenum, salt diagnostics, gas systems, controls, salt exchange tank, and *versatile*



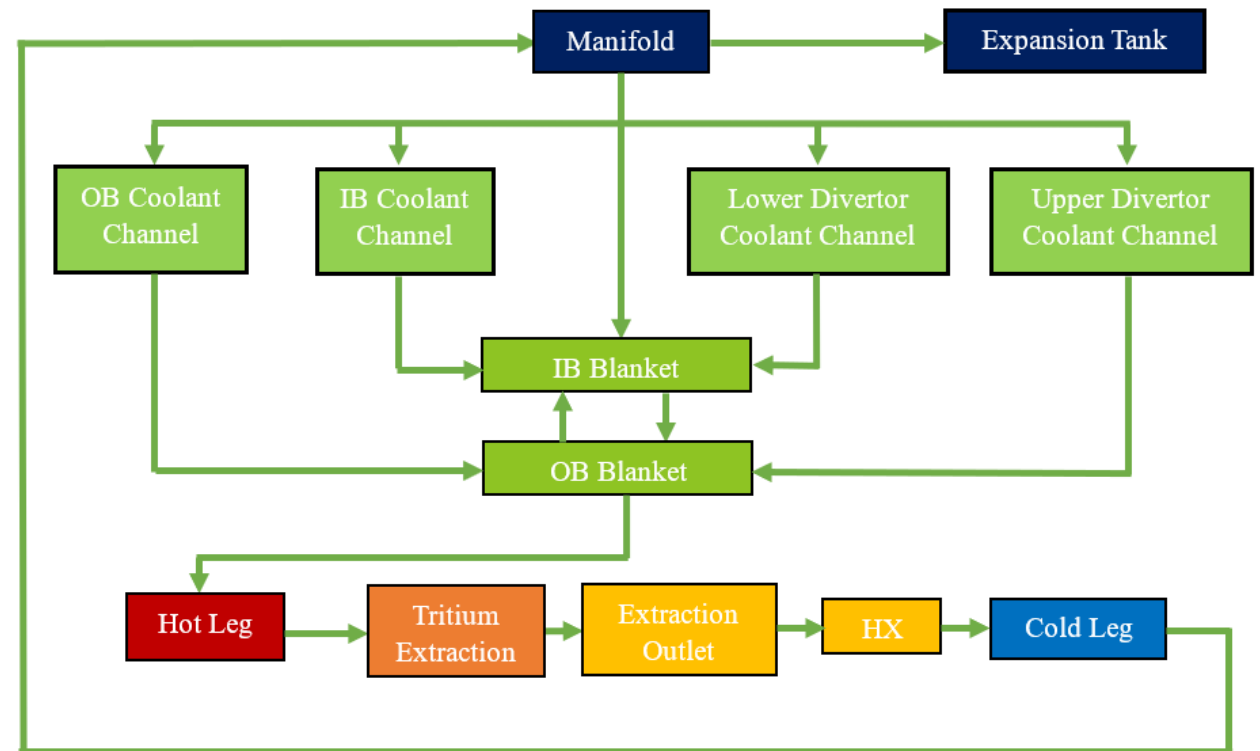
Liquid Immersion Blanket system setup

- Major components modeled in 1D simulation
- Divided into two sections, inboard and outboard
- Neutronics from MCNP analysis – plasma not modeled
- Coolant channels and blanket from vertically stacked CVs
- Tungsten split into three material types – First wall, near first wall and regular tungsten



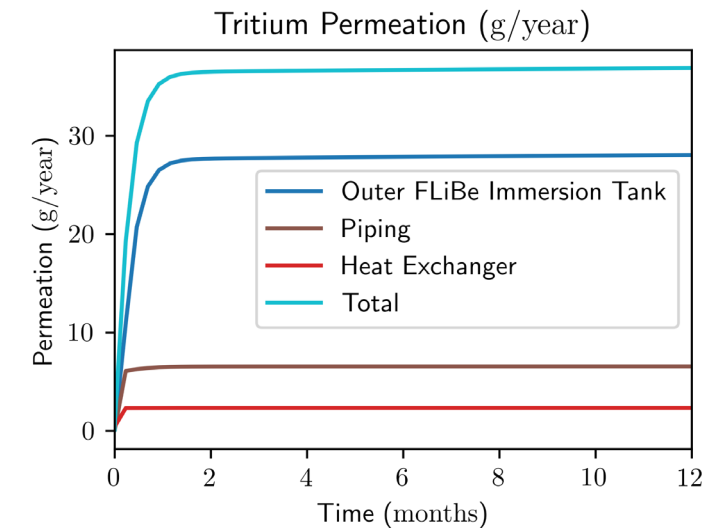
MELCOR system connections

- System operated as a closed-loop after steady-state was reached
- Tritium extraction system was modeled as a black box with an assumed efficiency positioned immediately prior to the heat exchanger system



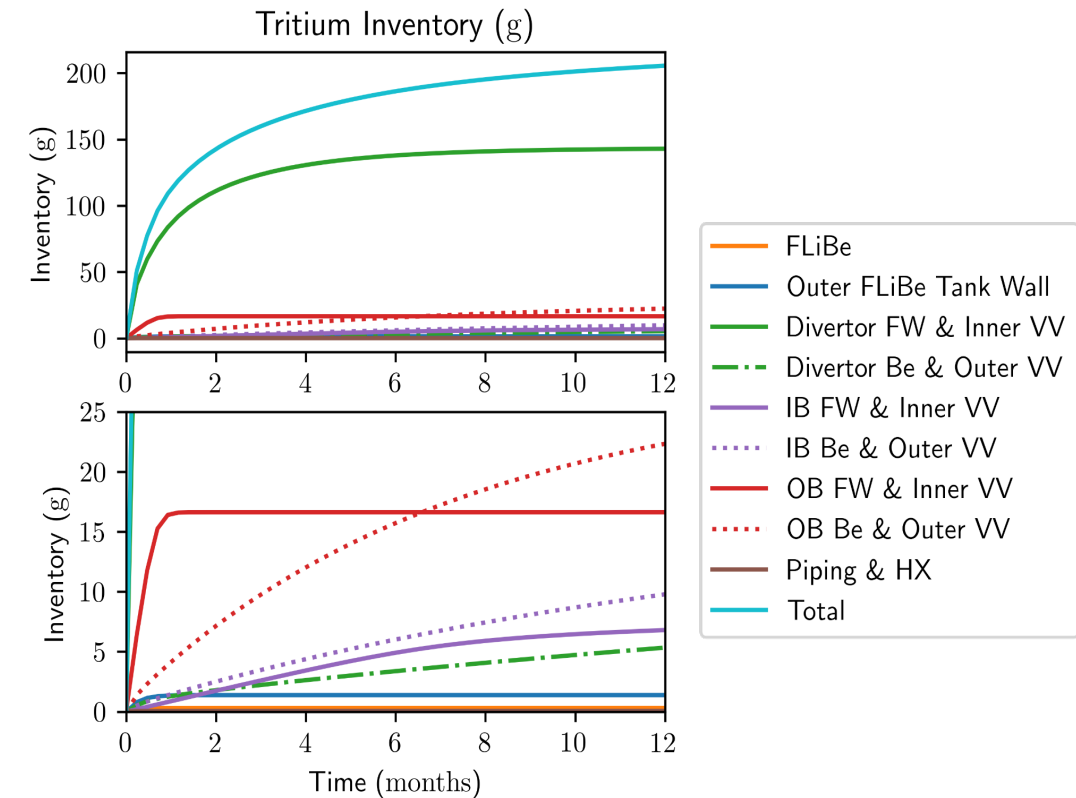
Tritium permeation

- All numbers are assuming 90% Tritium extraction system efficiency
- Permeation from the tank wall accounts for the majority of tritium migration at steady-state at 28 grams per year
- Pipes accounted for ~18% of tritium permeation
- A 100 μm tungsten permeation barrier was included, yielding a permeation rate of only 2.3 g/year tritium permeation through the heat exchanger in the base case



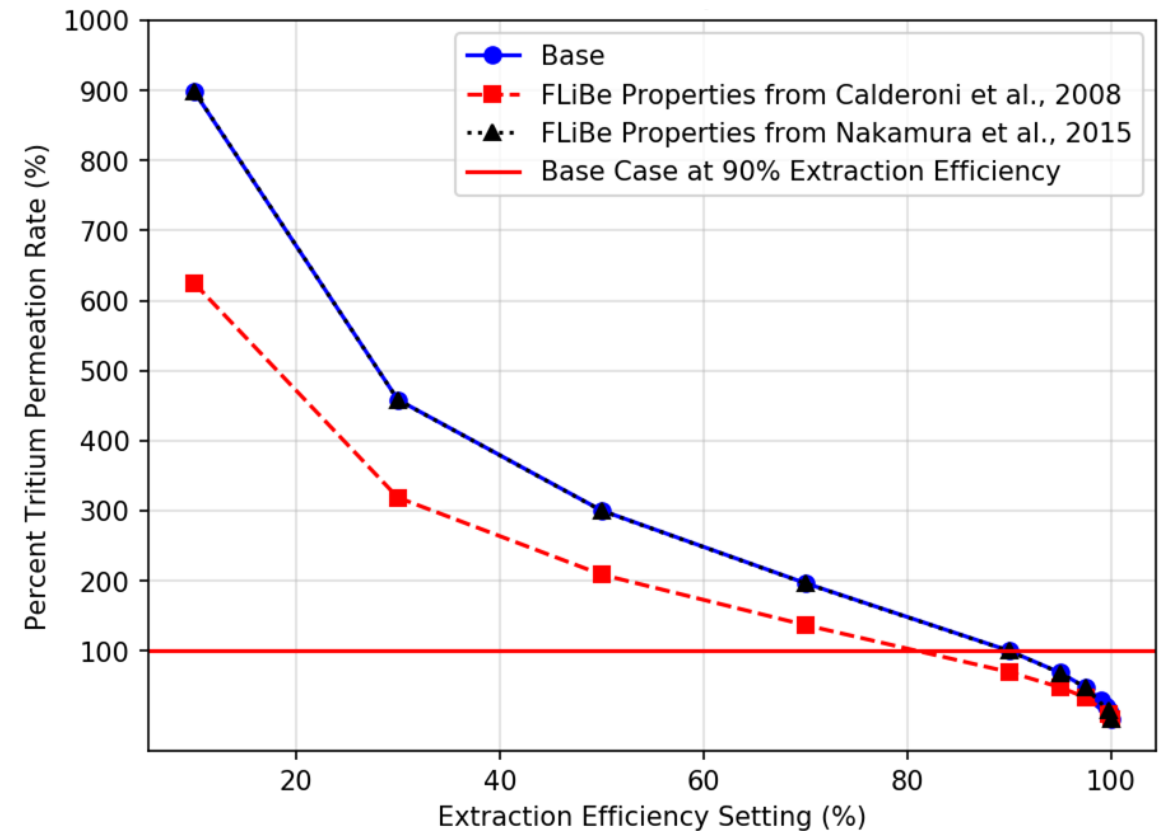
Steady-state tritium inventory

- Time to reach steady-state inventory was on the order of one year, not significantly different at two years (not shown)
- Total steady-state inventory was between 203 (10% TES efficiency) and 230 (99.99%) grams per year



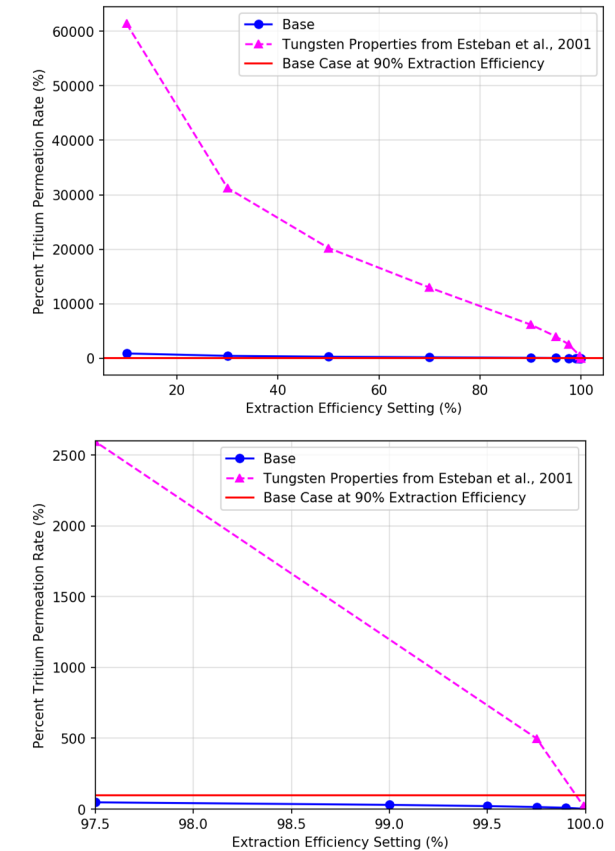
Tritium permeation rate as a function of TES efficiency

- Tritium extraction system modeled as black box having between 10 and 99.99% single pass efficiency
- Observed a 6-9x reduction in tritium permeation rate throughout the system at 90% single-pass efficiency compared to 10% efficiency base case



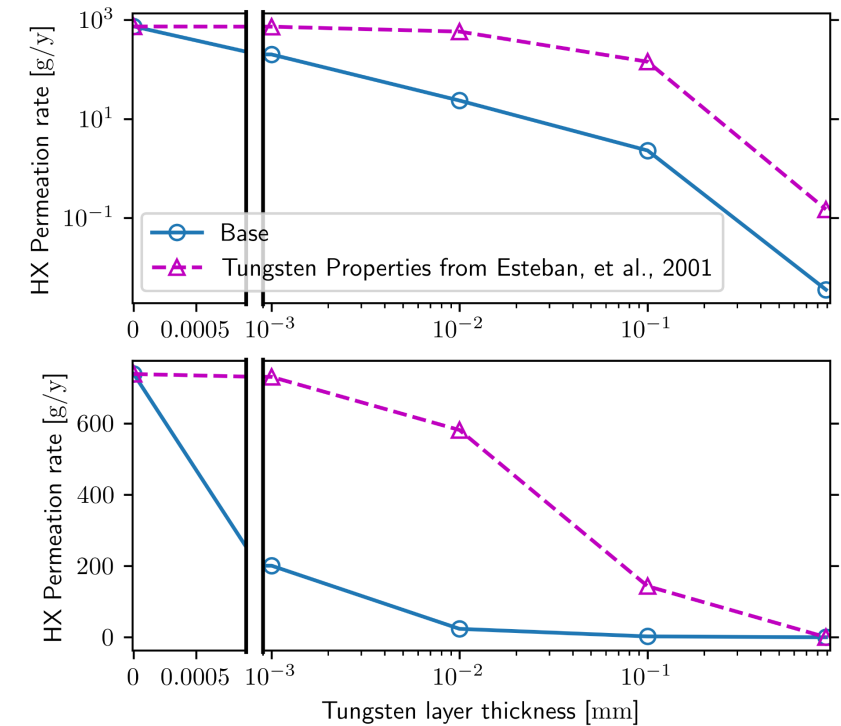
Permeation rate is much more sensitive to tungsten material properties than FLiBe diffusivities/solubilities

- Tungsten is used as a barrier layer
- The permeation of tritium in tungsten (within experimental uncertainties) has significant implications for design and tritium inventory management
- If tungsten material properties



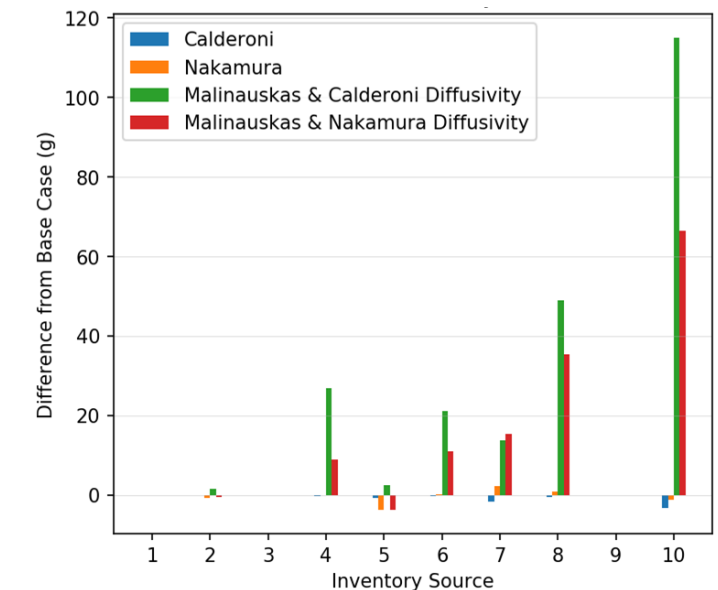
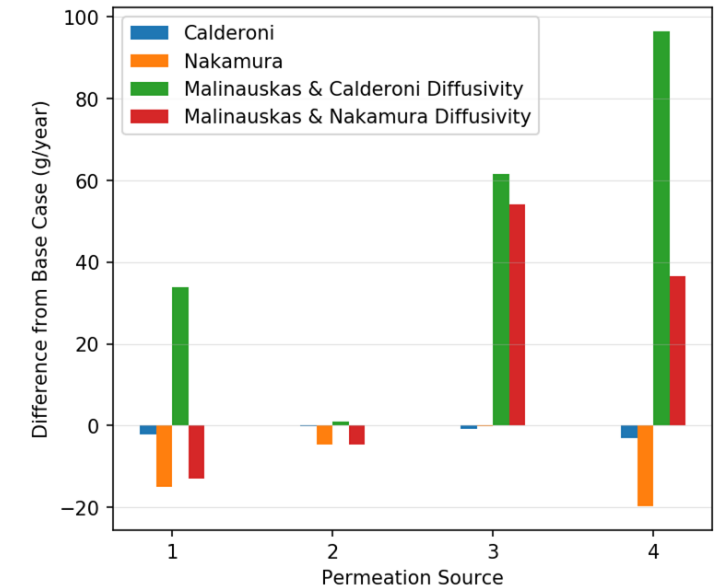
Tritium permeation as a function of HX wall coating thickness

- Composite heat exchanger wall design significantly reduces tritium transport through HX
- 0.1 mm width was chosen for base case

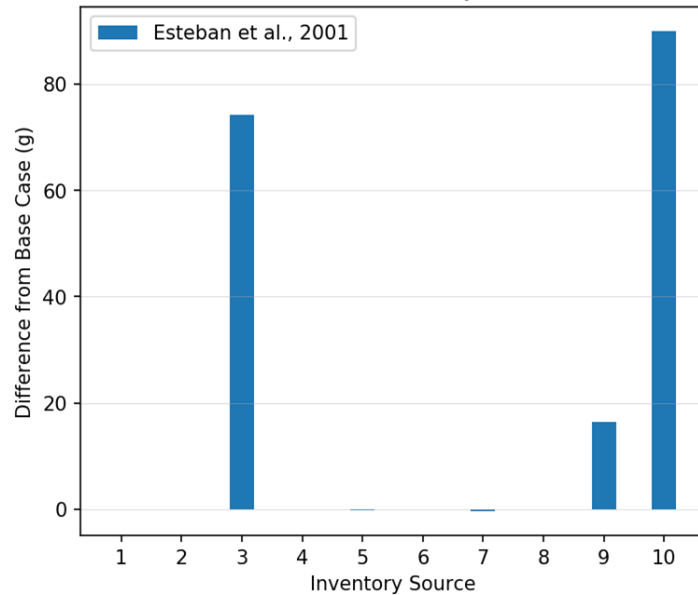


Permeation and inventory uncertainties remain due to uncertainties in material properties

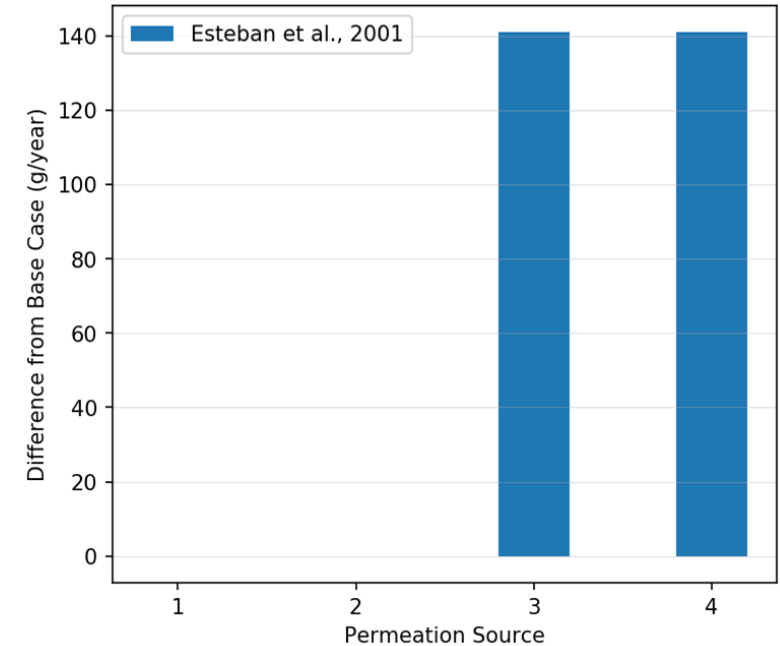
- Tritium solubility and diffusivity in FLiBe remains highly uncertain
- Comparison to regulatory limits and implications for fusion device classification



Tritium transport through tungsten is also uncertain



| Inventory Location | Location Label |
|--|----------------|
| FLiBe in Coolant & Blankets | 1 |
| Outer FLiBe Tank Wall | 2 |
| FW & Inner VV for Upper & Lower Divertors | 3 |
| Be Multiplier and Outer VV for Upper & Lower Divertors | 4 |
| IB FW & Inner VV | 5 |
| IB Be Multiplier & Outer VV | 6 |
| OB FW & Inner VV | 7 |
| OB Be Multiplier & Outer VV | 8 |
| Piping & HX Systems | 9 |
| Total | 10 |



| Permeation Location | Location Label |
|---|----------------|
| Outer FLiBe Immersion Tank Wall | 1 |
| Pipes | 2 |
| Heat Exchanger w/ 100 um W permeation barrier | 3 |
| Total | 4 |

Conclusions

- Permeation through an ARC class device is most highly sensitive to the material properties of the barrier layer
- Liquid blanket tritium permeability has smaller, but still comparable implications on tritium inventory management
- The tritium extraction system is limited in its ability to mitigate total device tritium permeation losses
- Experimental apparatuses under development and in testing phase will allow tighter constraints on material properties used in future modeling

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