INL/MIS-24-79856-Revision-0

Modeling with Tritium Accountancy Using MELCOR Fusion

July 2024

Changing the World's Energy Future

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Idaho National Laboratory

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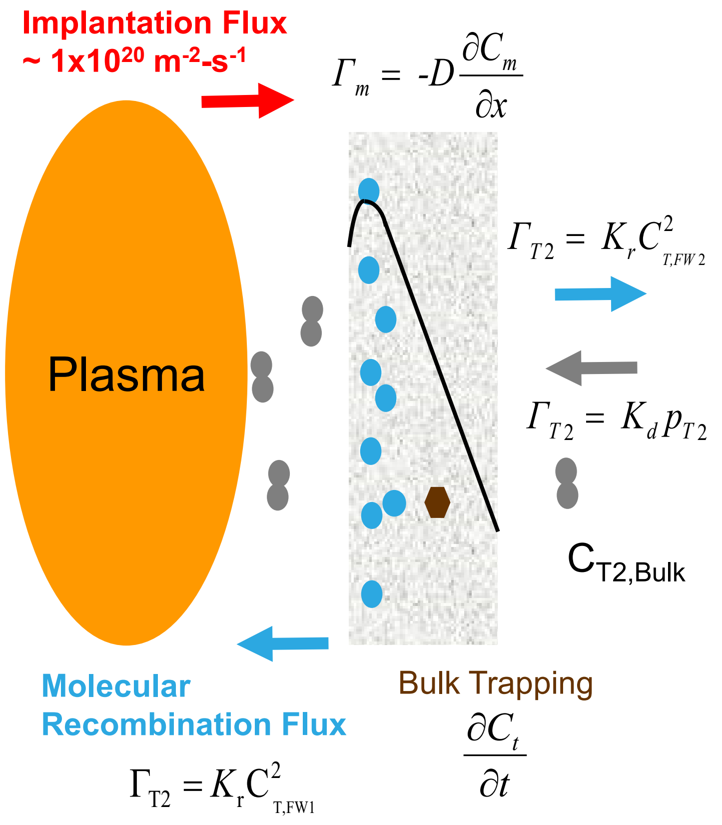
Fusion Safety Overview

- 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

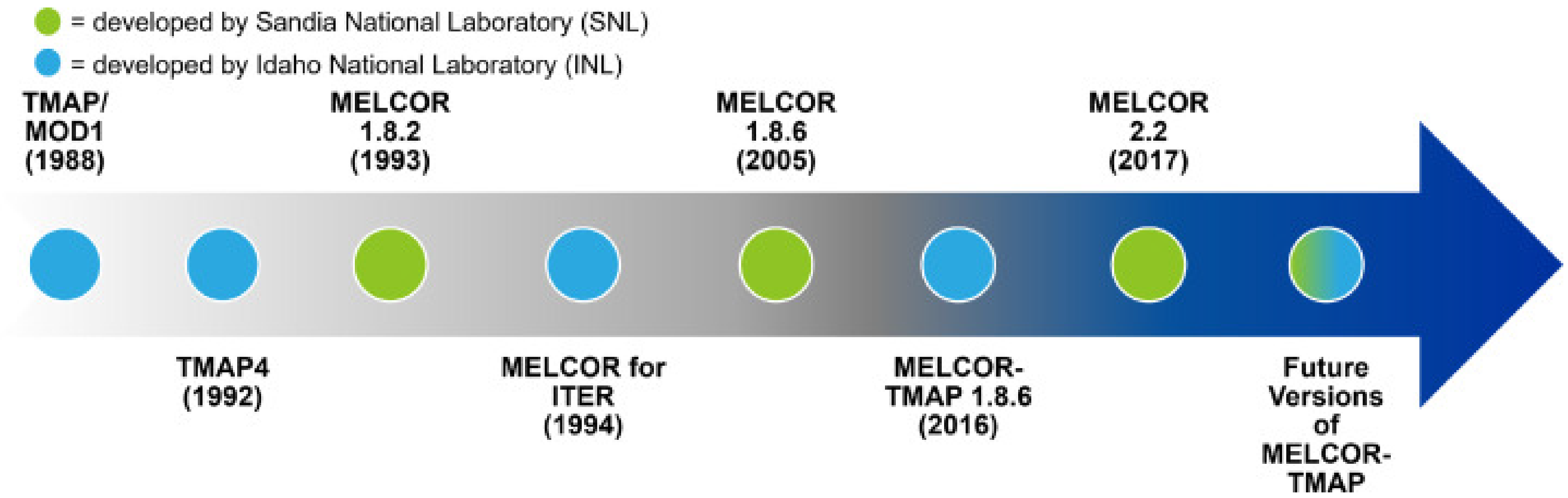
TMAP

- 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



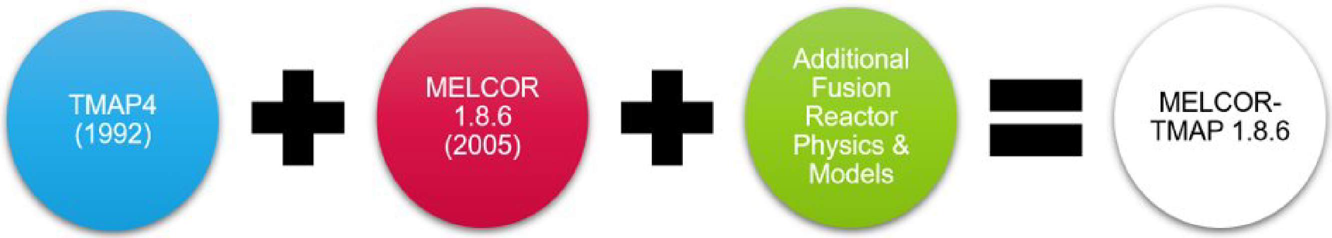
History of MELCOR-Fusion

- 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

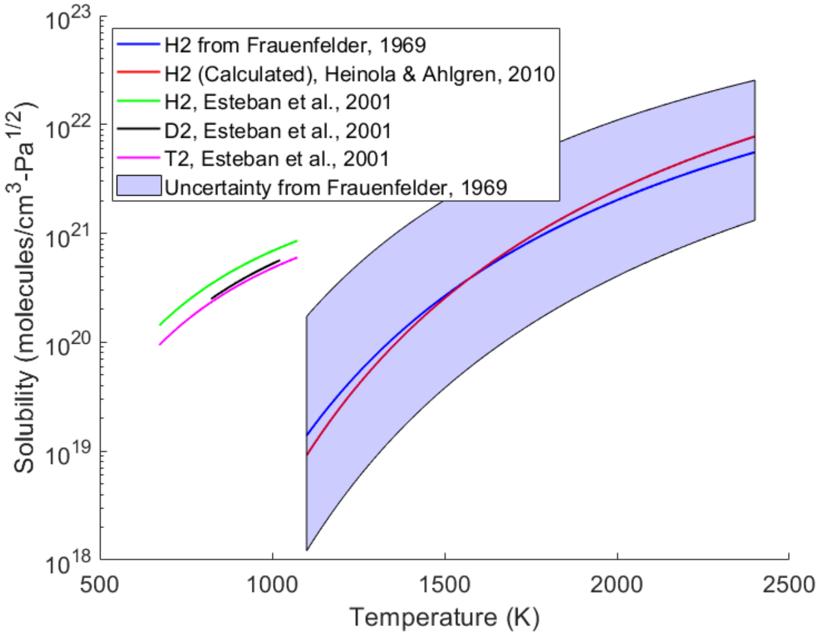
- Heat transfer
- Thermal hydraulics
- Vapor & aerosol tracking
- Reactor accidents

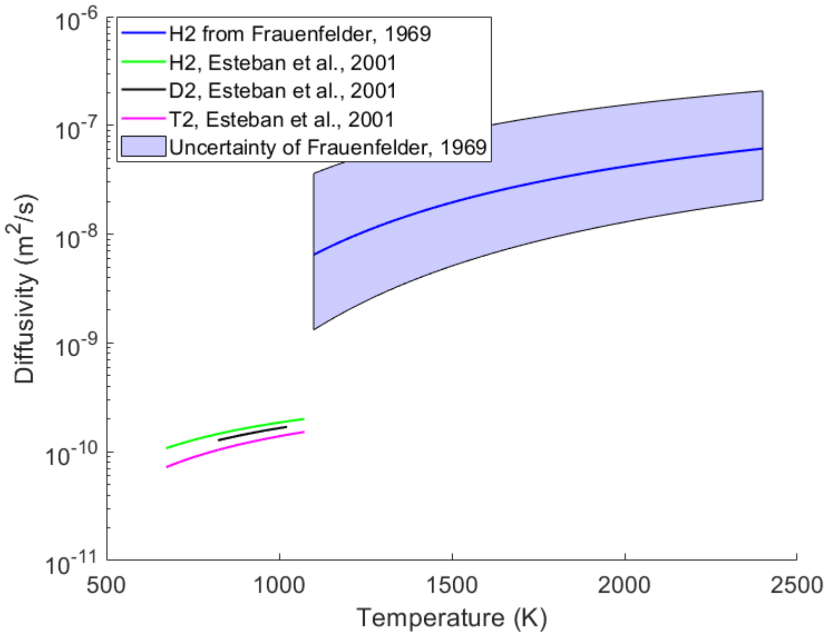
- HTO modeling
- Lithium fire accidents
- Multiple working fluids

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

Tritium transport through tungsten is uncertain

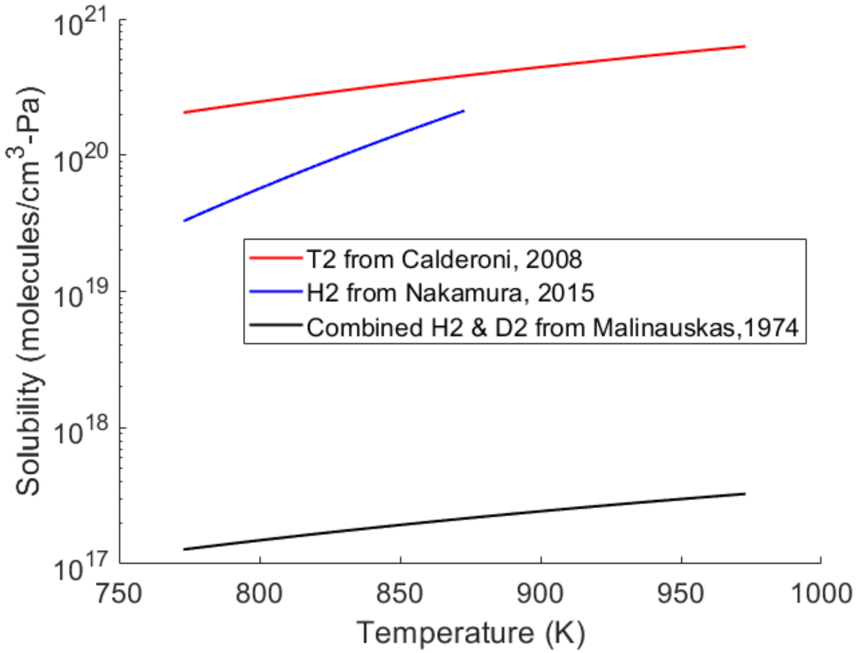
- Estimates of solubility of tritium in tungsten vary by three orders of magnitude
- Estimates of tritium diffusivity in tungsten vary by four orders of magnitude
- We take Frauenfelder's 1969 material properties for our base case

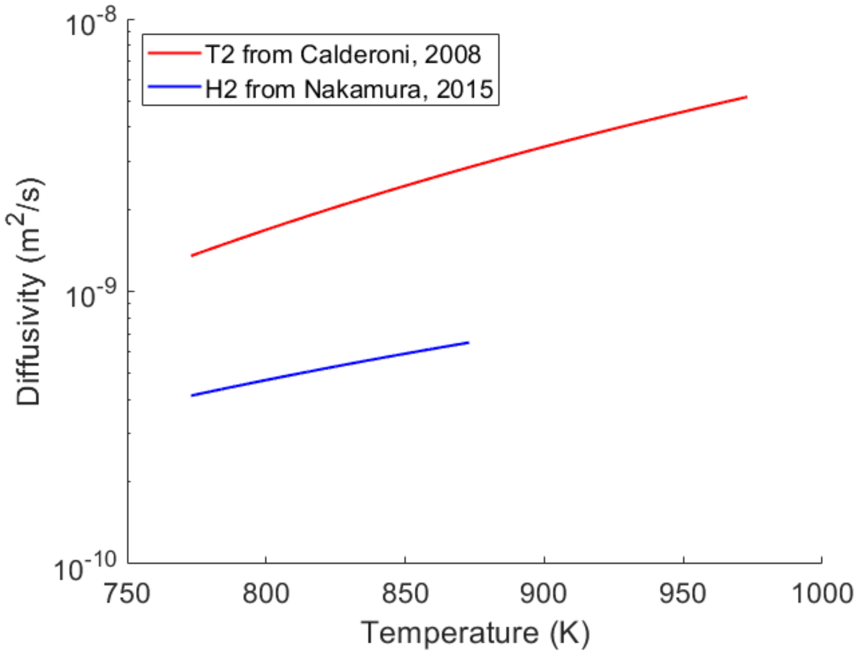




Experimental work on tritium transport in FLiBe

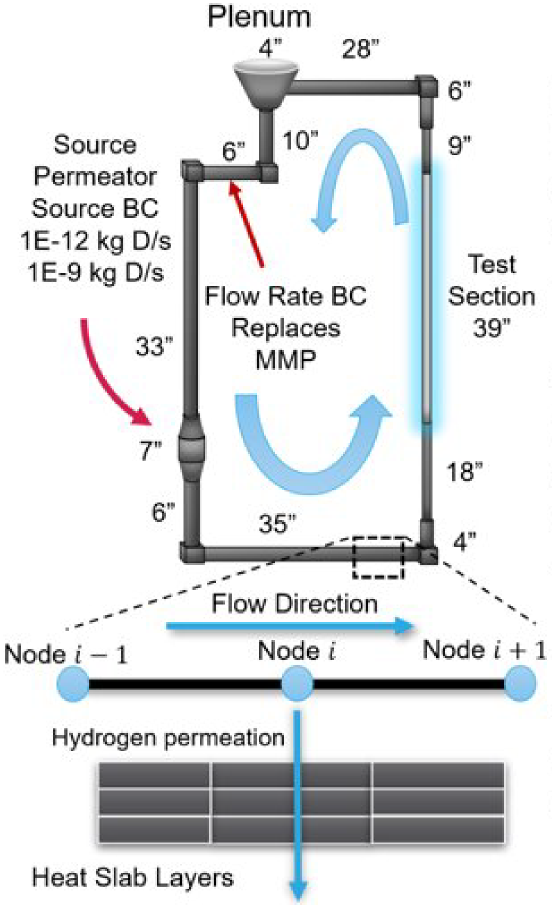
- There is a lack of experimental data on the solubility and diffusivity of tritium in FLiBe
- Existing data shows several orders of magnitude uncertainty
- We take Calderoni's 2008 work for our base case





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



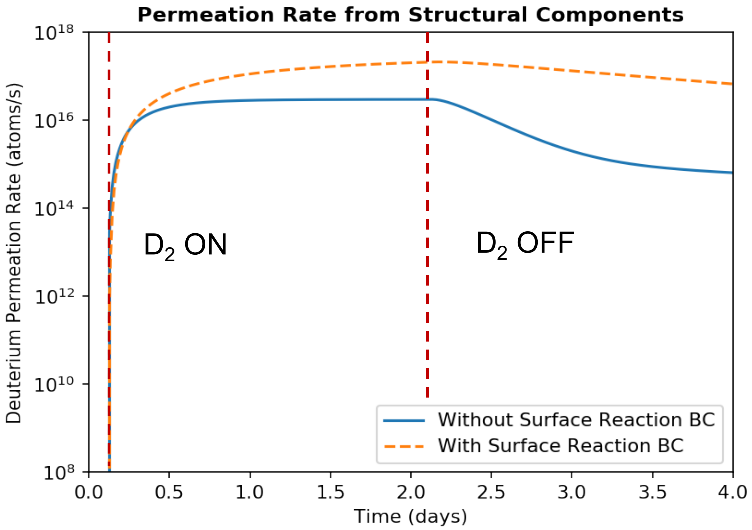
Primary Tubing Specs (316 SS)
- OD: 1”
- ID: 0.87”
- Wall thickness: 0.065”

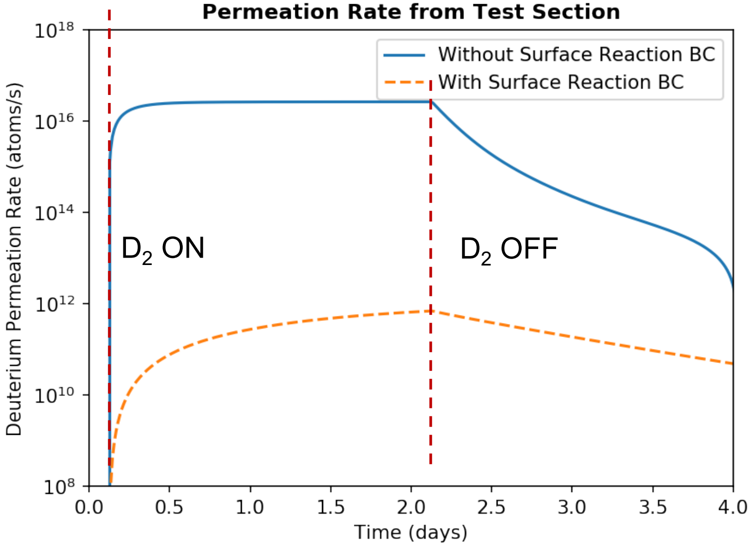
Secondary Tubing Specs (316 SS)
- OD: 0.5”
- ID: 0.37”
- Wall thickness: 0.065”

Test Section (Vanadium)
- OD: 0.5”
- ID: 0.46”
- Wall thickness: 0.02”

MELCOR-TMAP Simulations

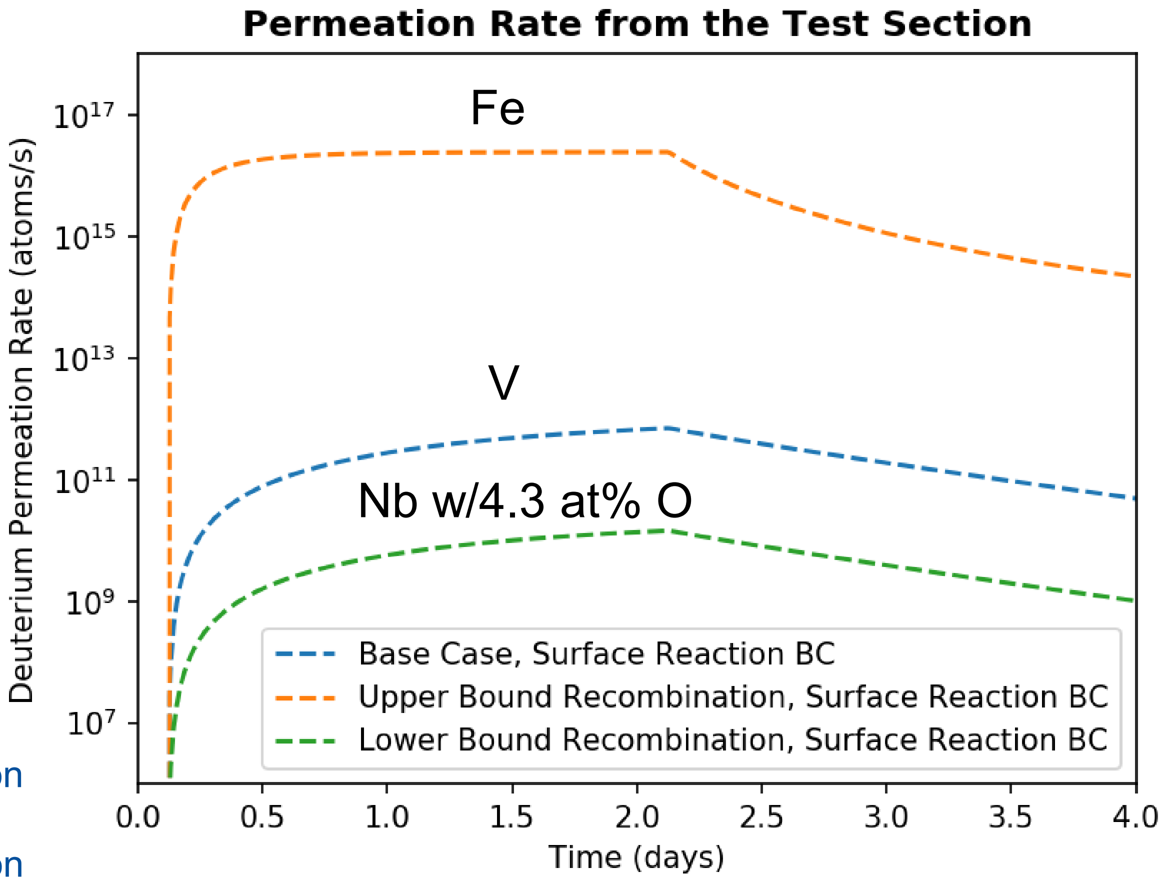
- Deuterium source:
  - Source boundary condition: 3e+17 atom/s source term, 48 hours ON and 48 hours OFF
- Permeation rates and transient behavior depend on boundary conditions applied (solution law vs. surface reaction rates)
- Surface-reaction BC accounts for:
  - Recombination of deuterium on the 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 bound[1]: Fe recombination
  = 5.9e-27*exp(-0.20/kT) m^4·molecule/(s·$atom^2$)
  - Nominal case[2]: V recombination
  = 7.6e-25*exp(-1.32/kT) m^4·molecule/(s·$atom^2$)
  - Lower bound[3]: Nb with 4.3 at% O
  = 2.6e-30*exp(-0.81/kT) m^4·molecule/(s·$atom^2$)
- Results demonstrate permeation rate is highly sensitive to recombination of permeator material, ranging in ~6 orders of magnitude from lower to upper bounds



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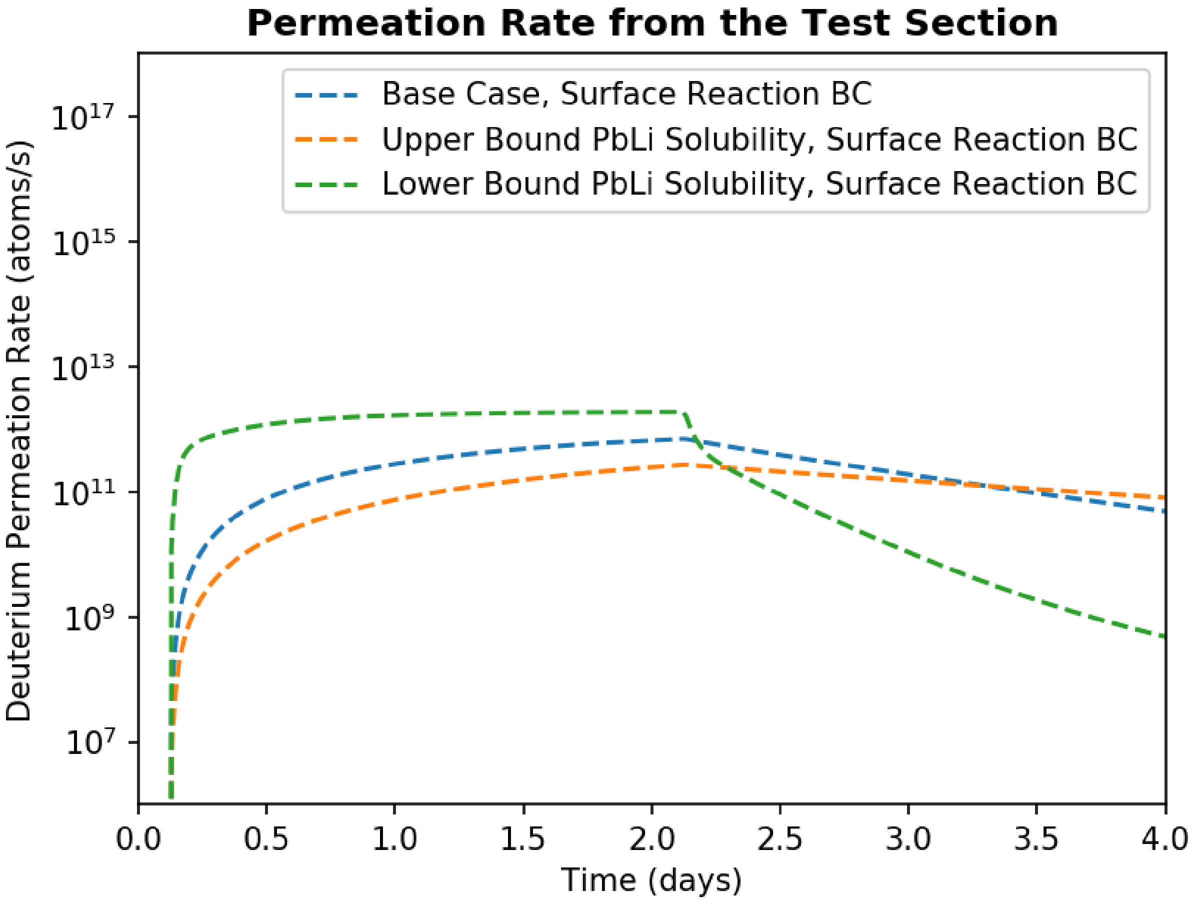
Sensitivity to PbLi Solubility

- PbLi solubility modified:
  - Upper bound[1]

    = 3.6e+22 atoms/($m^3 \cdot Pa^{1/2}$)
  - Nominal case[2]

    = 1.4e+23*exp(-0.13/kT) atoms/($m^3 \cdot Pa^{1/2}$)
  - Lower bound[3]

    = 7.7e+20*exp(-0.01/kT) atoms/($m^3 \cdot Pa^{1/2}$)
- Results show solubility affects rate of change in permeation rate, but doesn't greatly affect the SS permeation value



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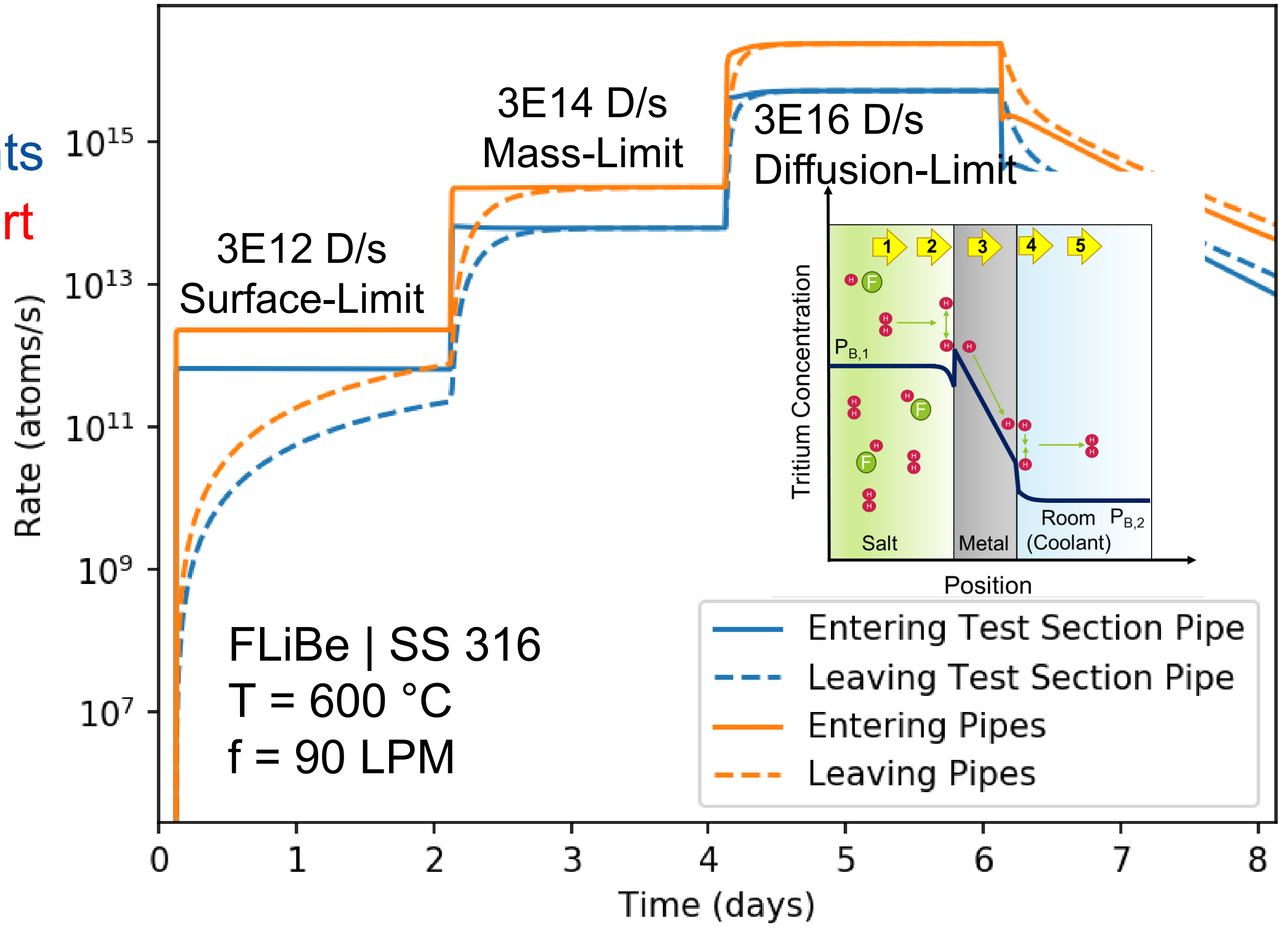
Experimental Campaigns

- 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]



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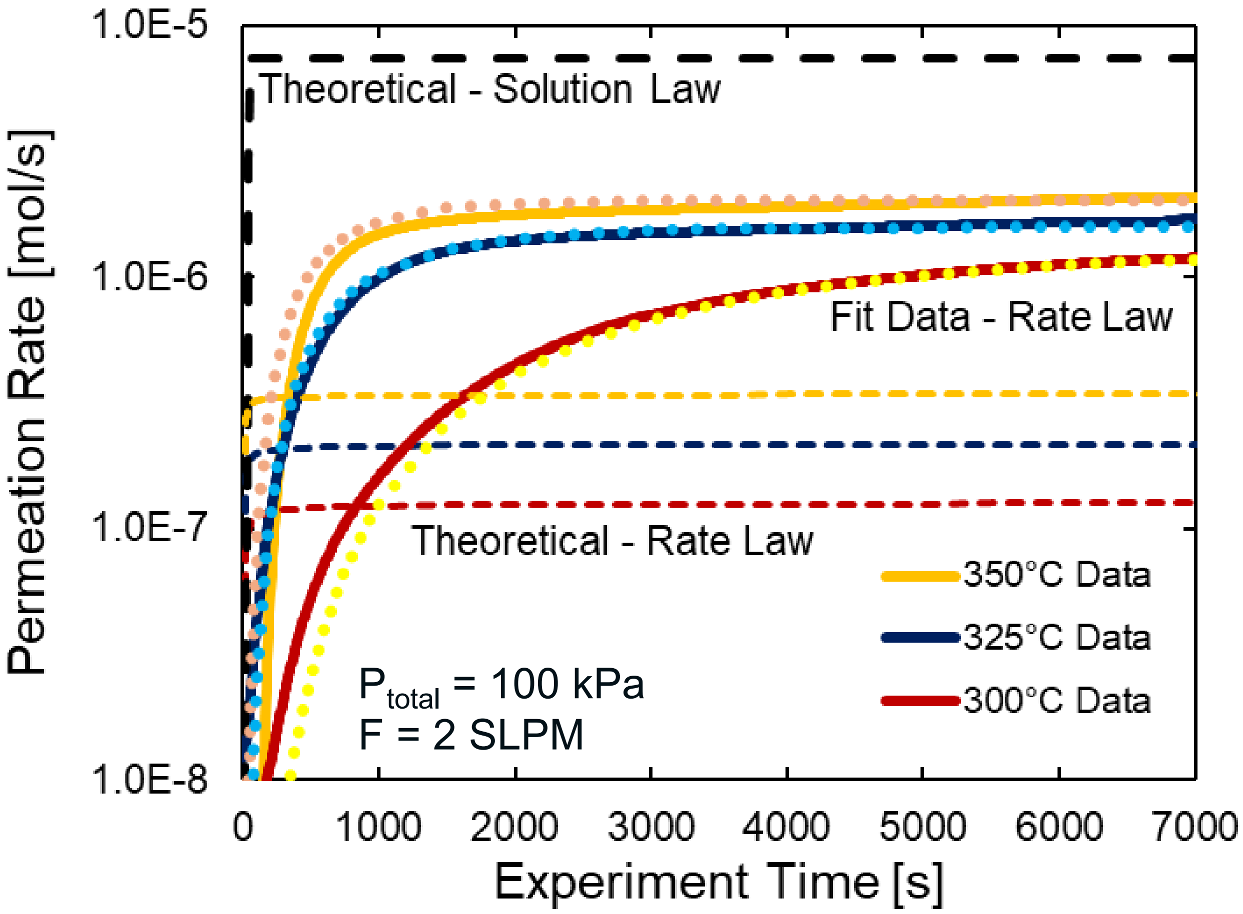
MELCOR-TMAP TEX Model

- Deuterium Transport Properties
  - **D**: 2.05E(-4.20/RT) $m^2\ s^{-1}$ [1]
  - **Ks**: 0.138E(29.0/RT) mol $m^{-3}\ Pa^{-0.5}$ [2]
  - **k_R**: 1.30E(-127/RT) $m^4\ mol^{-1}\ s^{-1}$ [3]
- **Solution law** (Sieverts') BC overpredicts.
- **Rate law** (Surface rxn) BC underpredicts.
- **Fit Data**: *increase* **k_R** by factor of ~12, and *decrease* **D** by factor of ~100.
- Decreased apparent permeability consistent with experimental observations [3].
- Increased k_R also consistent with recent experiments [4].



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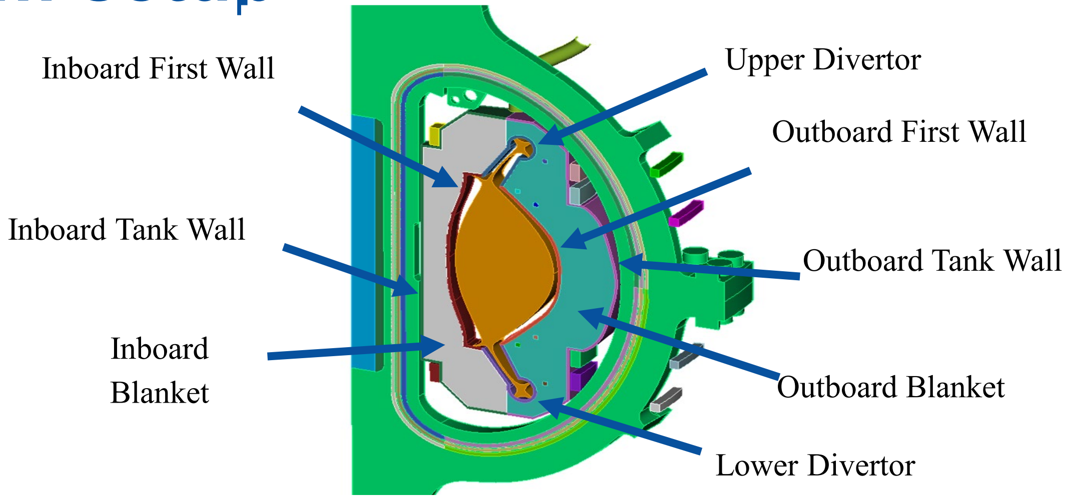
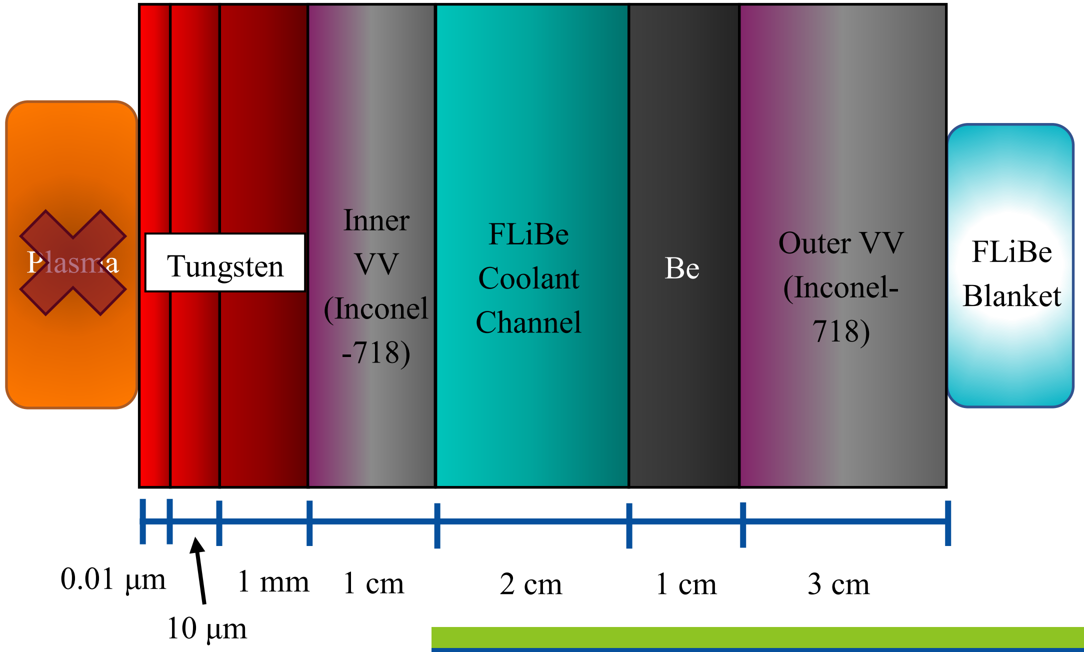
Liquid Immersion Blanket system setup

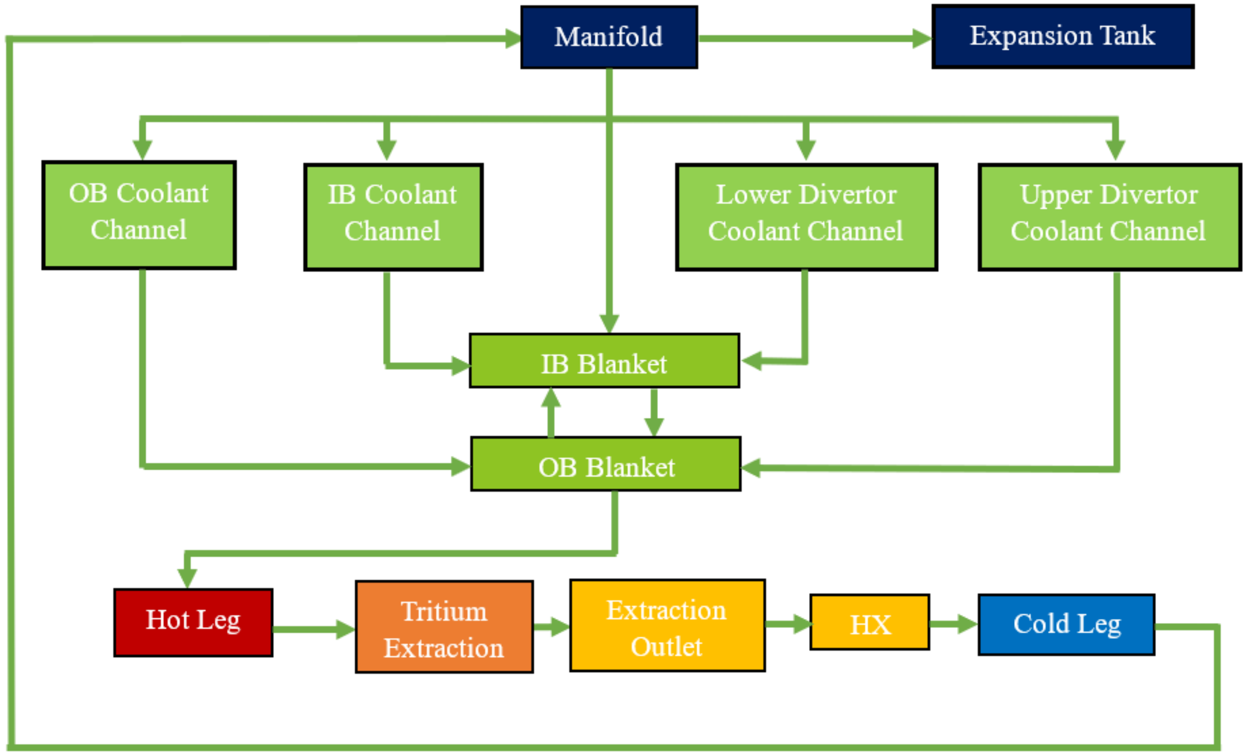
- Major components modeled in 1D simulation
- Divided into two sections, inboard and outboard
- Neutronics from MCNP analysis – plasma not modeled
- Coolant channels and blanket from vertically stacked CVs
- Tungsten split into three material types – First wall, near first wall and regular tungsten





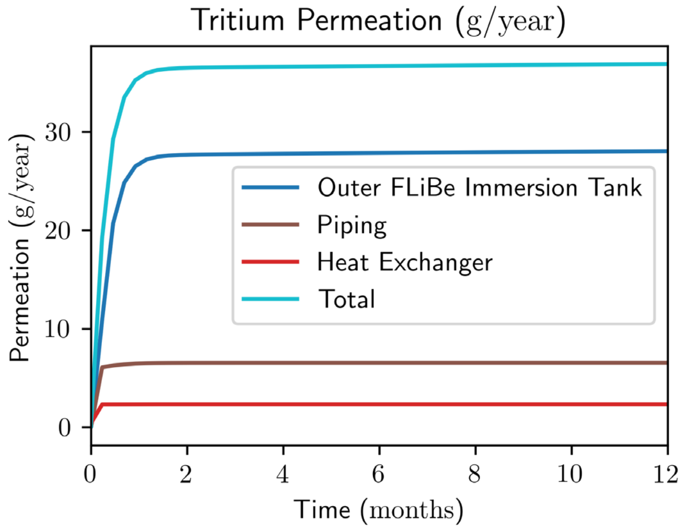
MELCOR system connections

- 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



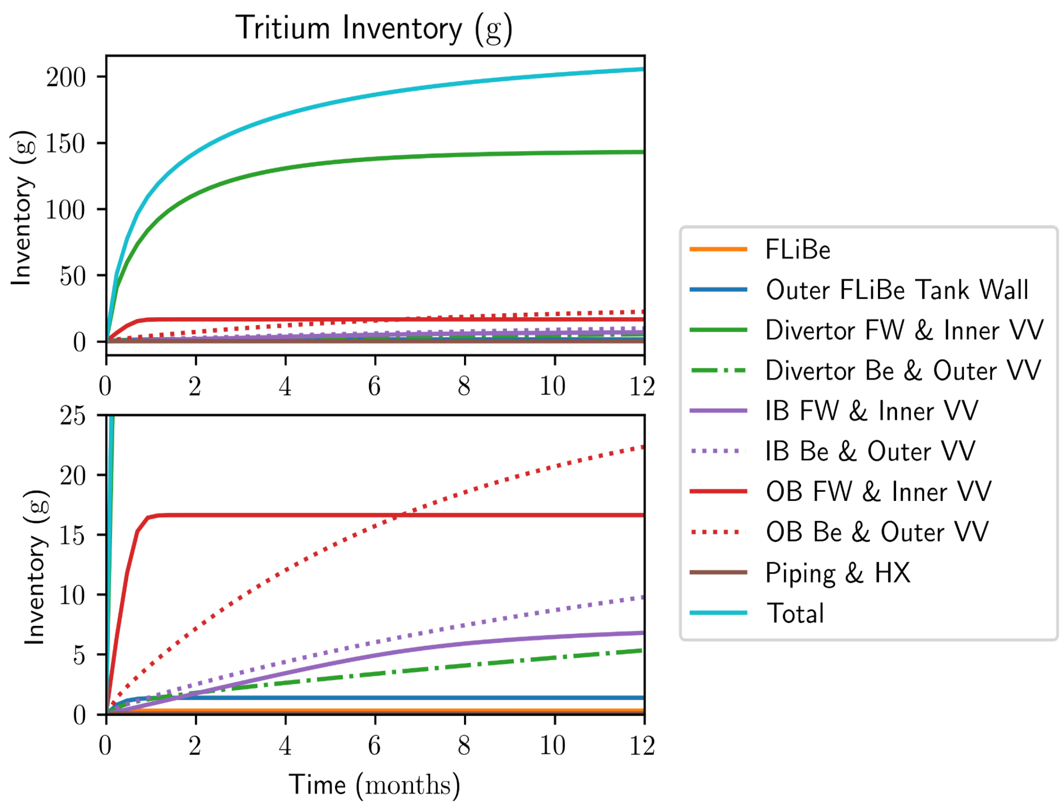
Tritium permeation

- 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



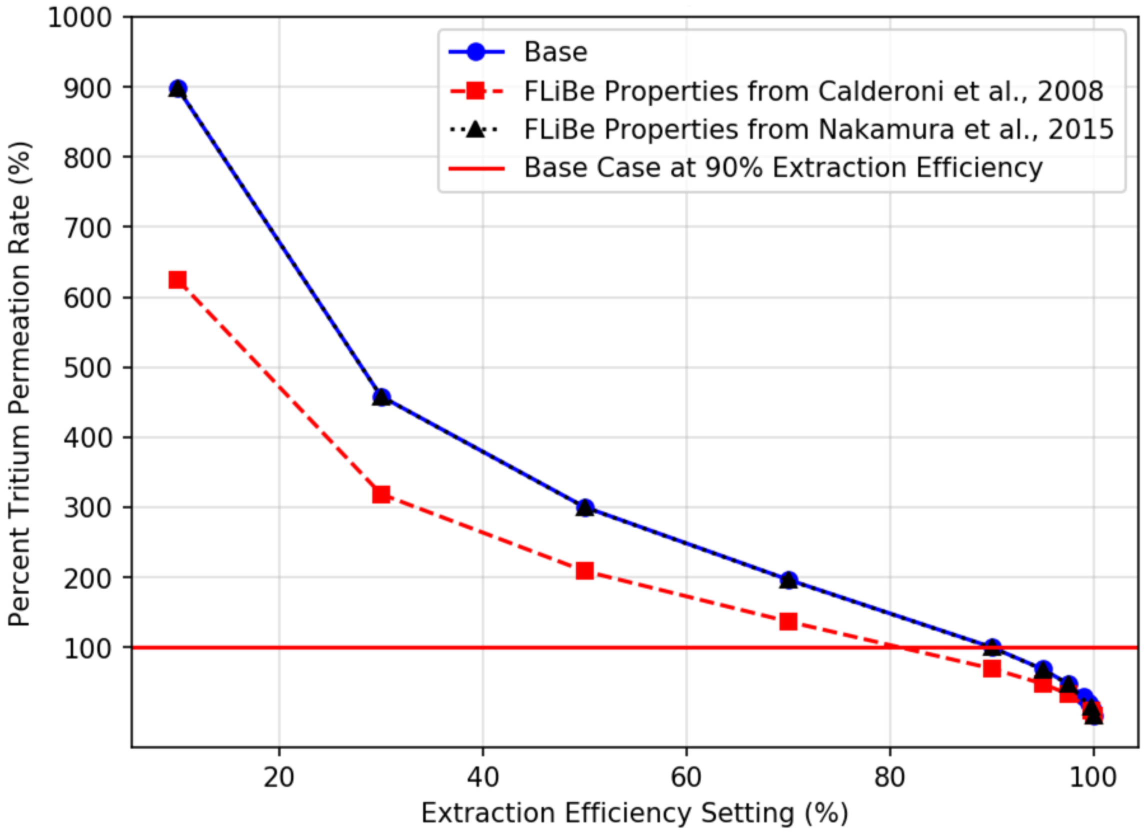
Steady-state tritium inventory

- Time to reach steady-state inventory was on the order of one year
- Total steady-state inventory was between 203 (10% TES efficiency) and 230 (99.99%) grams per year



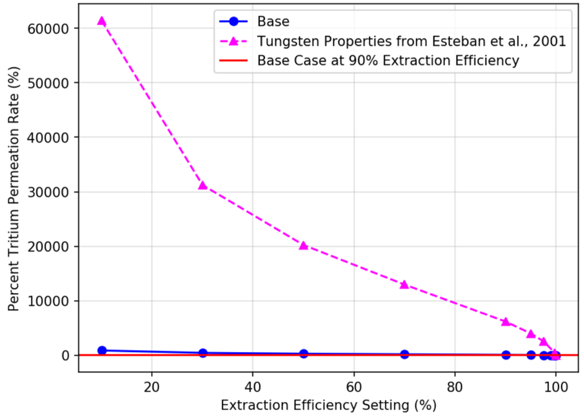
Tritium permeation rate as a function of TES efficiency

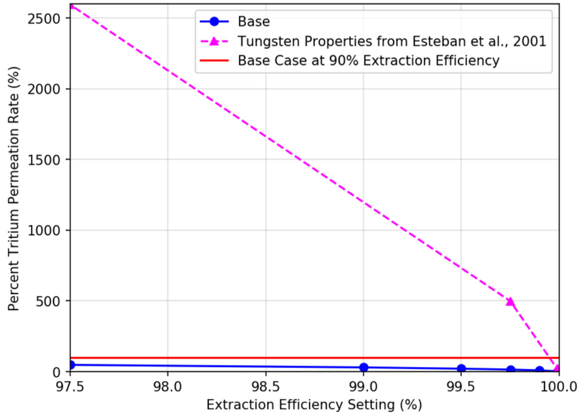
- Tritium extraction system modeled as black box having between 10 and 99.99% single pass efficiency
- Observed a 6-9x reduction in tritium permeation rate throughout the system at 90% single-pass efficiency compared to 10% efficiency base case



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

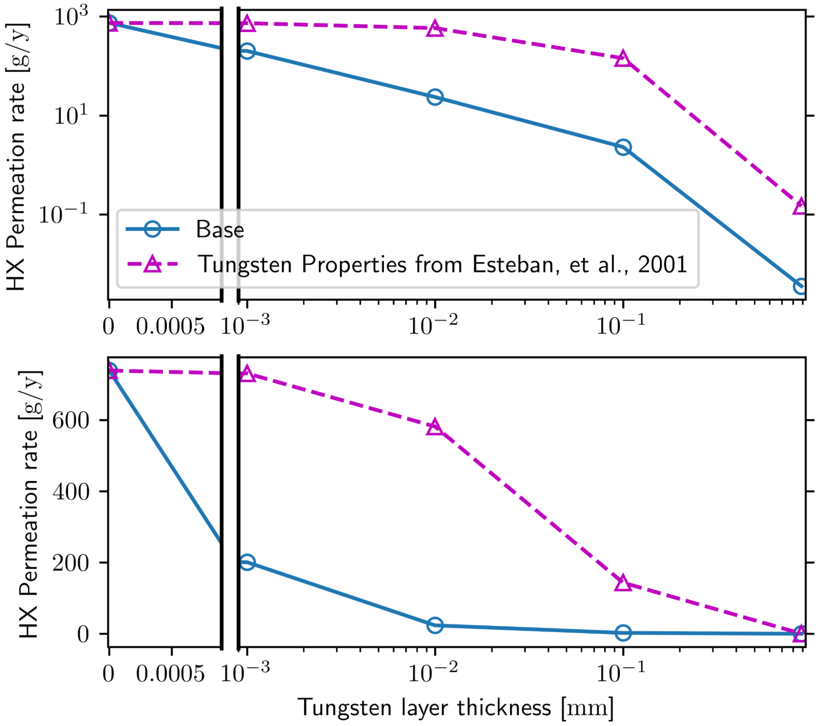
- Tungsten is used as a barrier layer
- The permeation of tritium in tungsten (within experimental uncertainties) has significant implications for design and tritium inventory management
- If tungsten material properties





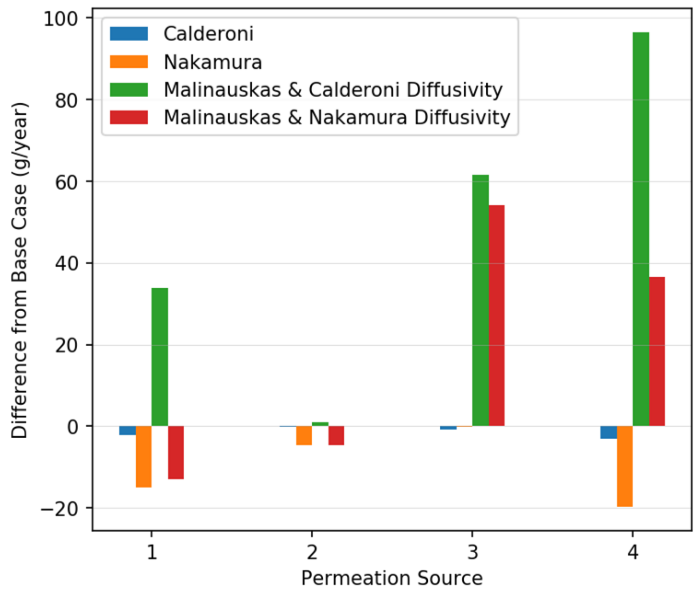
Tritium permeation as a function of HX wall coating thickness

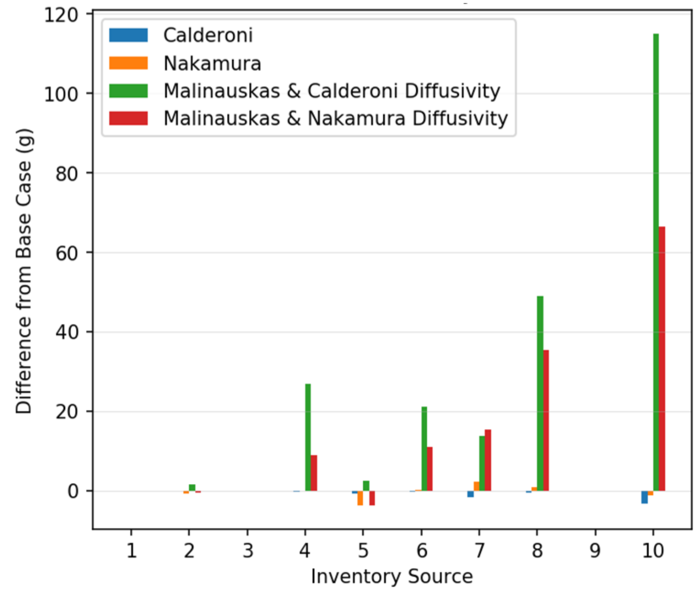
- Composite heat exchanger wall design significantly reduces tritium transport through HX
- 0.1 mm width was chosen for base case



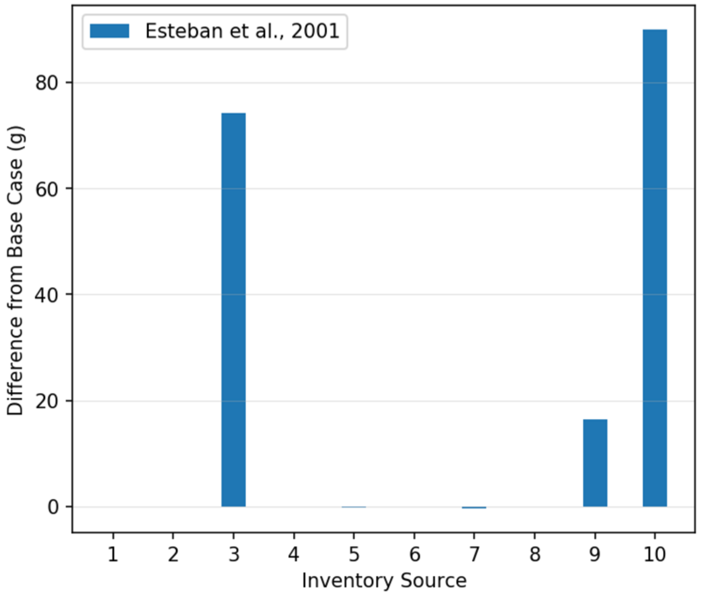
Permeation and inventory uncertainties remain due to uncertainties in material properties

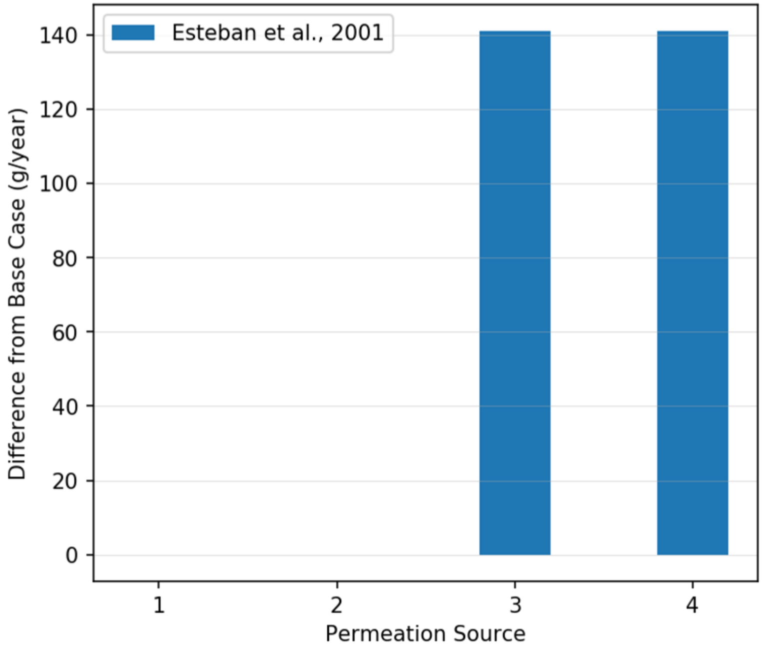
- Tritium solubility and diffusivity in FLiBe remains highly uncertain
- Comparison to regulatory limits and implications for fusion device classification





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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