



SOFE2023 Presentation: "Tritium Safety and Sensitivity Analysis of Tritium Extraction eXperiment (TEX) PbLi Loop Using MELCOR- TMAP"

Changing the World's Energy Future

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July 2023

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



SOFE 2023

— **OXFORD, UK** —

30TH IEEE SYMPOSIUM ON
FUSION ENGINEERING



Tritium Safety and Sensitivity Analysis of Tritium Extraction eXperiment (TEX) PbLi Loop Using MELCOR-TMAP

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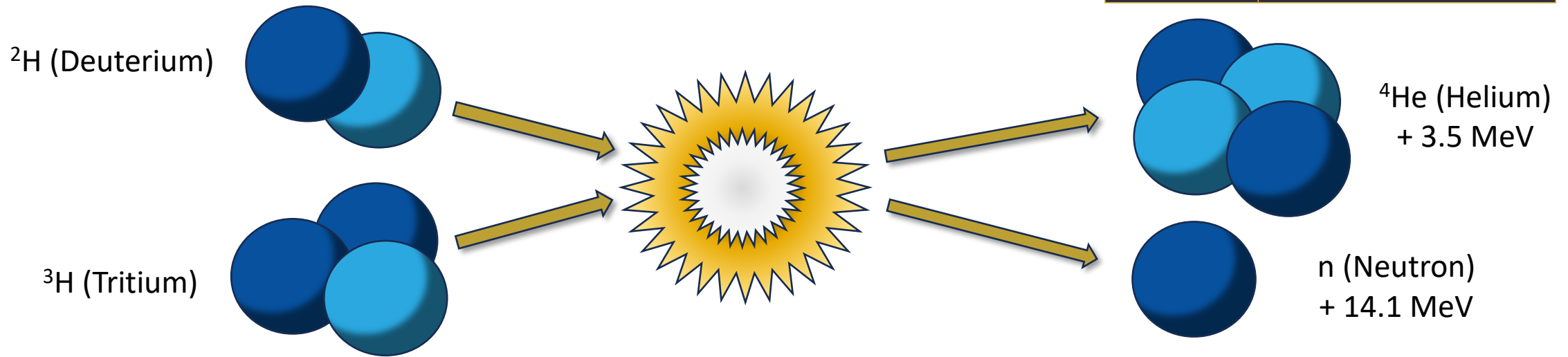


Outline

- Background
- Tritium Extraction eXperiment (TEX)
- MELCOR-TMAP
- TEX Model in MELCOR-TMAP
- MELCOR-TMAP Simulations
- Conclusions & Future Work



Background



- Tritium supply is a crucial consideration for the design of a self-sustaining fusion power plant
- Breeding & extraction of tritium from the coolant and/or breeder in the vacuum vessel is a main area of focus in fusion reactor science & engineering

Background



- Among liquid & solid breeder concepts, the lead-lithium eutectic alloy, Pb-15.72Li, or PbLi, is a leading candidate for liquid breeder blanket designs
- Efficient extraction systems for liquid breeders will limit permeation & release of radioactive tritium & provide tritium for continuous reactor operation

Background



Method	Description	Benefits	Issues
Gas-Liquid Contactor	Packed column, liquid-gas sparging system.	<ul style="list-style-type: none">• Mature technology• Planned in ITER	<ul style="list-style-type: none">• Large system• High energy consumption/low eff.
Vacuum Sieve Trays	Jet of droplets. T ₂ evolves from droplet into vacuum.	<ul style="list-style-type: none">• High efficiency• Simplicity	<ul style="list-style-type: none">• Low flexibility with PbLi flowrate• High uncertainty, risk, and pressure drop
Regenerable Getters	Tritium gettering bed using high solubility materials.	<ul style="list-style-type: none">• Compact• High efficiency	<ul style="list-style-type: none">• Requires regeneration• High tritium inventory
Vacuum Permeator	Permeable membrane. Vacuum on secondary side.	<ul style="list-style-type: none">• Continuous/simple• High efficiency	<ul style="list-style-type: none">• Membrane stability• High capital costs – large surface area

Utili, Marco, et al. "Tritium Extraction From HCLL/WCLL/DCLL PbLi BBs of DEMO and HCLL TBS of ITER." IEEE Transactions on Plasma Science 47.2 (2019): 1464-1471.

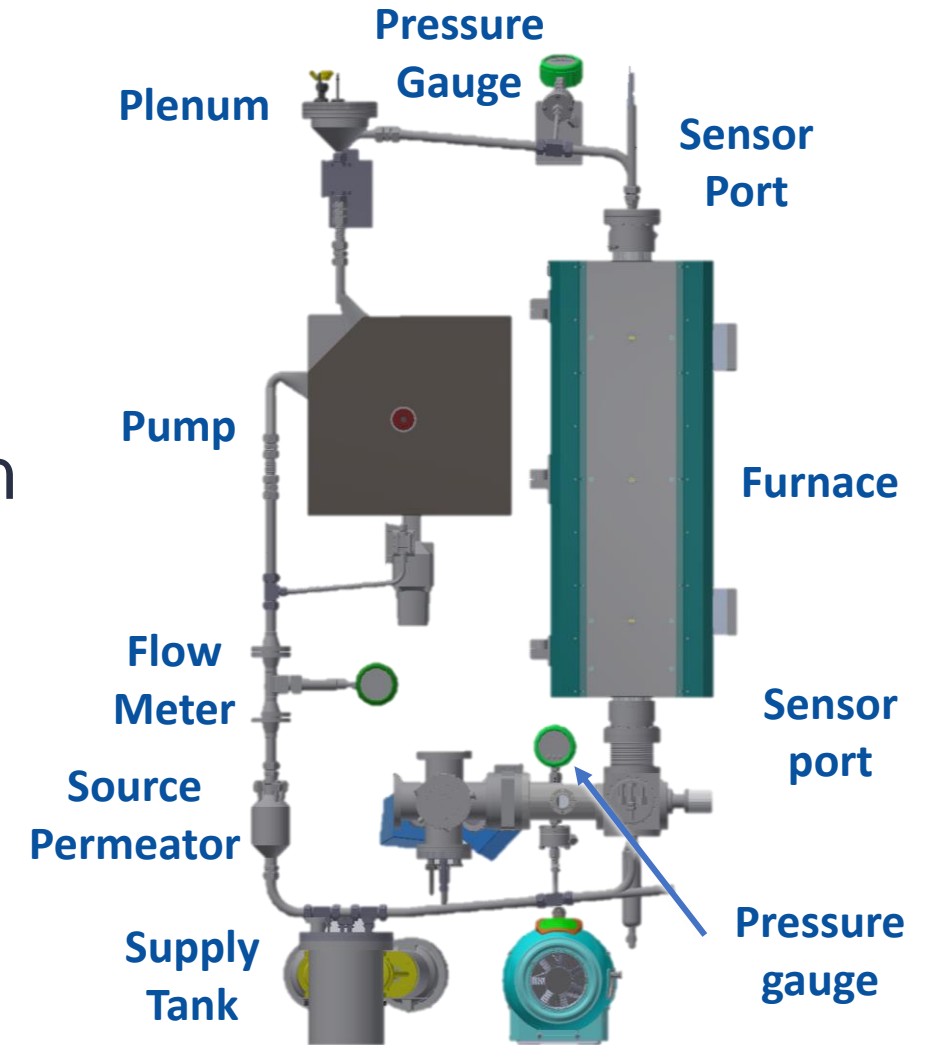
Tritium Extraction eXperiment (TEX)



- The Tritium Extraction eXperiment (TEX) in development at the Safety and Tritium Applied Research (STAR) Facility at Idaho National Laboratory (INL) includes a forced-convection PbLi loop designed to extract tritium using a vacuum permeator, one of several leading concepts for extracting tritium from PbLi breeders
- Goal for TEX is to test & measure the effectiveness of the vacuum permeator concepts for extracting tritium from PbLi. The versatile test stand is capable of testing multiple configurations and permeator materials.

Tritium Extraction eXperiment (TEX)

- Source permeator designed to inject hydrogen (deuterium, tritium) into the PbLi
- Furnace surrounds the test section to maintain the test section at a fixed temperature
- Vacuum is pumped outside the test section permeator tube. Hydrogen permeates through the permeator tube and the rate is measured with calibrated Quadrupole Mass Spectrometers



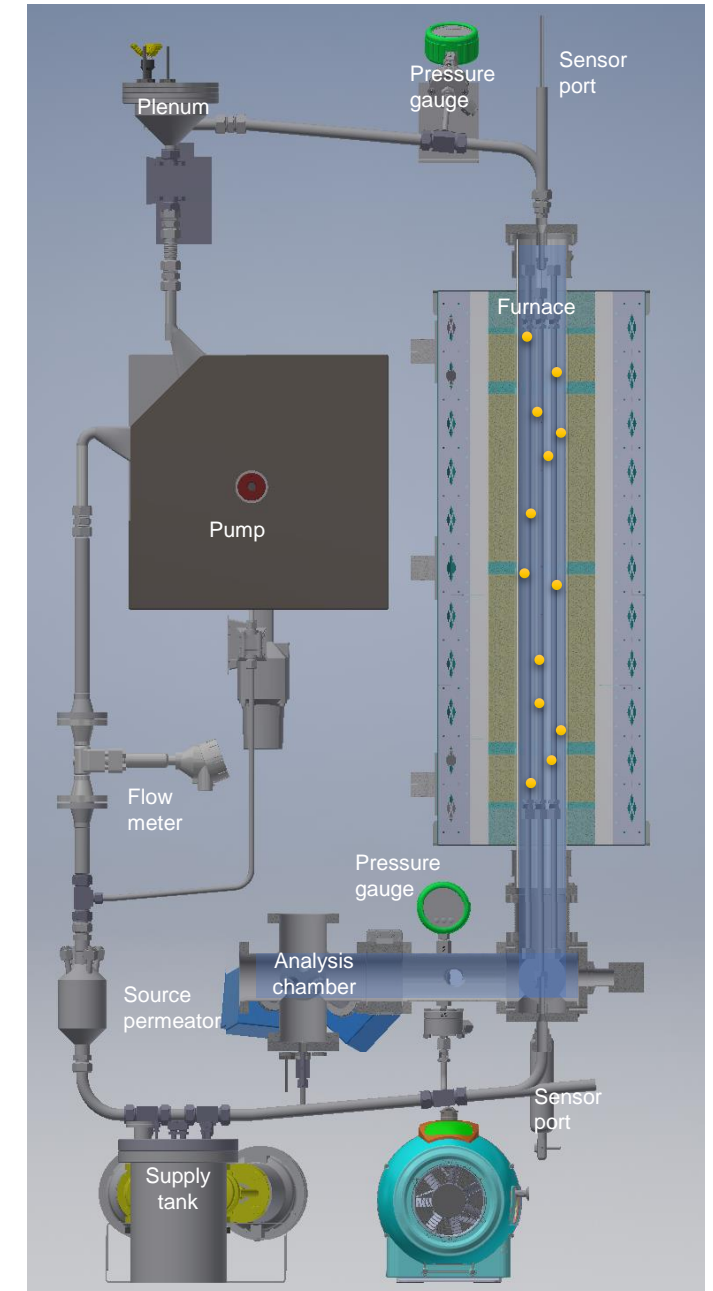
Tritium Extraction eXperiment (TEX)

- Unique features:
 - Interchangeable/expandable test section
 - Access for testing additional diagnostics
 - Ability to use tritium

Parameter	TEX	Blanket Concepts		
		DCLL	WCLL	HCLL
Flow rate (max)	0.5 L/s 4.7 kg/s	26000 kg/s	956 kg/s	890 kg/s
Permeator length	1-5 m			
Temperature	300-535°C	535°C	311.5°C	300°C
D concentration (mol/m ³)	$\leq 2 \times 10^{-2}$	5.56×10^{-4}	1.41×10^{-2}	6.61×10^{-3}
Tritium capable	Yes	Yes	Yes	Yes

[1] M. Utili, et al., IEEE Trans. Plasma Sci. 47 (2019) 1464–1471

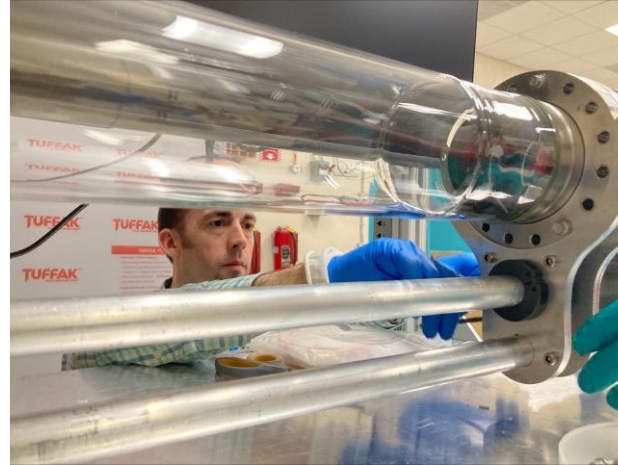
[2] B. Garcinuño, et al., Fusion Eng. Des. 137 (2018) 427–434



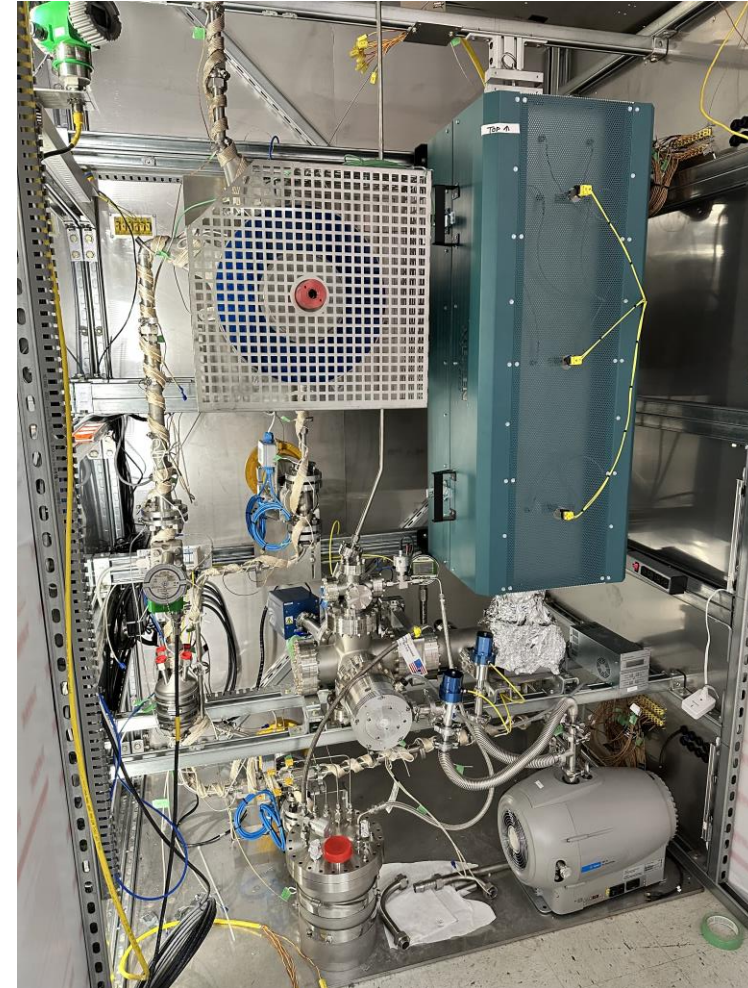
Tritium Extraction eXperiment (TEX)



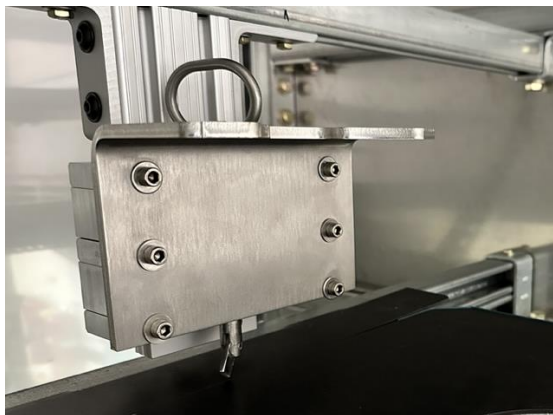
Installation complete of
HEPA exhaust blower



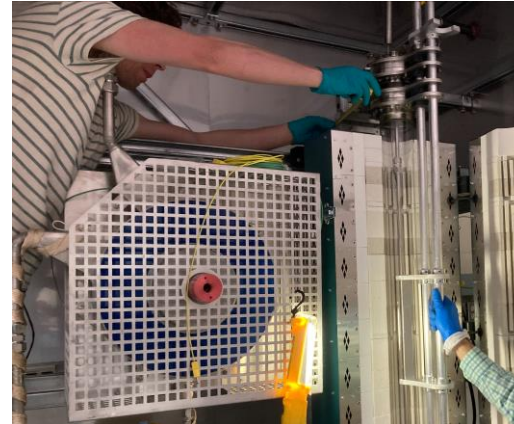
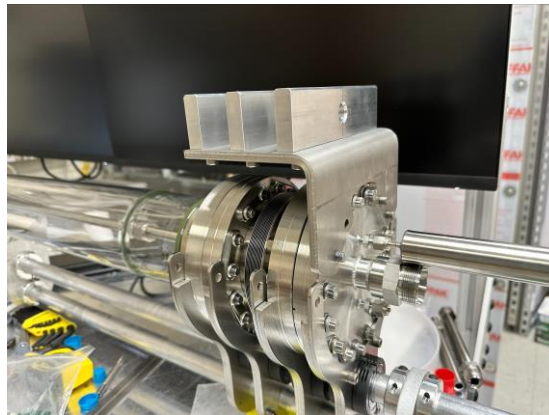
Installation of mockup tube into test section housing



Current view of TEX



Test section support track



Installation of test section into loop

Steady-State Tritium Transport Model

- PbLi flows inside tube, vacuum on shell side
- T diffuses through wall and collected by vacuum
- Steady-state 1D radial T flux (J):

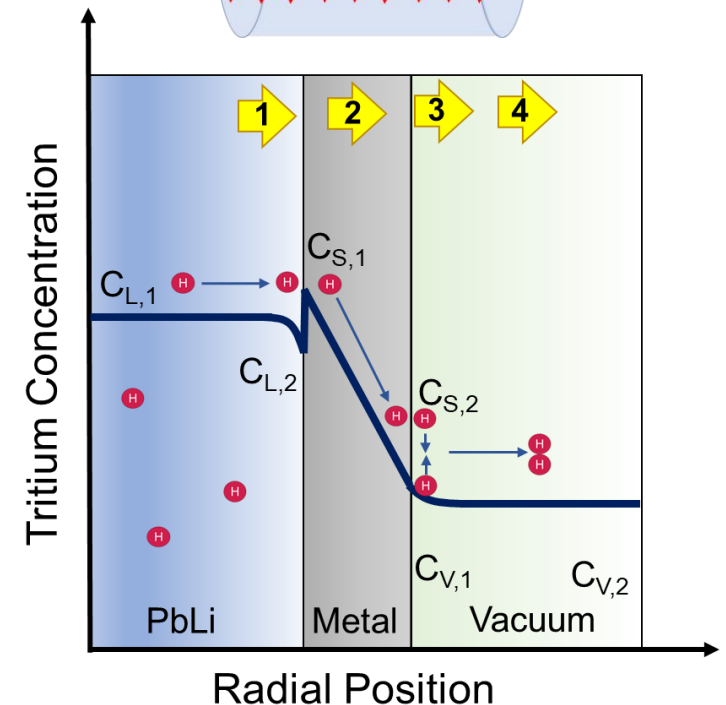
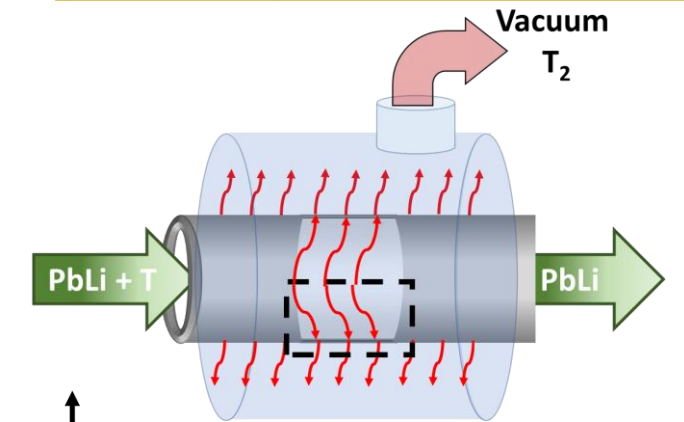
1. Mass transfer in PbLi: $J = k_{T,1}(C_{L,1} - C_{L,2})$

2. Diffusion through metal: $J = -D_S \frac{\partial C_S}{\partial r}$

3. Recombination: $J = k_r C_{S,2}^2 - k_d P_{V,1}$

4. ~~Mass transfer vacuum: $J = k_{T,2}(C_{V,1} - C_{V,2})$~~

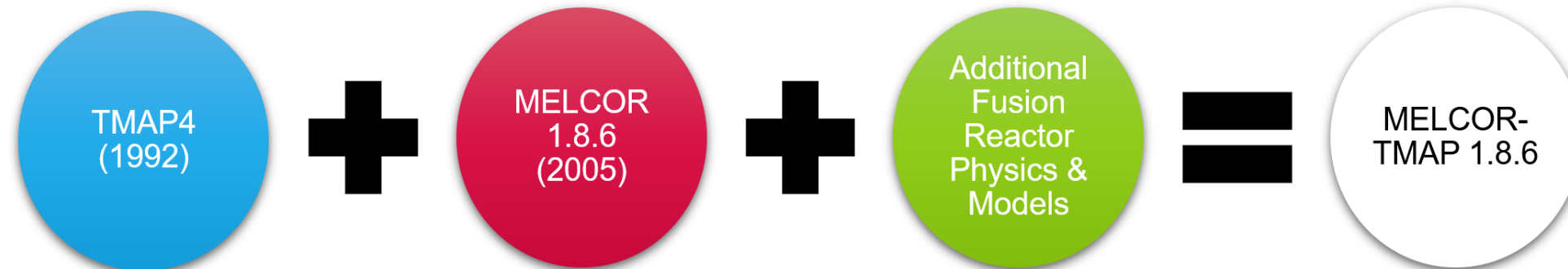
- Models are only as accurate as the input parameters... which can encompass significant uncertainty.



MELCOR-TMAP



- Part of the safety analysis for TEX includes modeling & simulation of the experiment loop using MELCOR-TMAP, owned & developed by the Fusion Safety Program at INL
- MELCOR-TMAP (latest version 1.8.6) is a system-level engineering code based on MELCOR and TMAP4 for hydrogen species transport & safety analysis for fusion reactors & related technologies



- | | | | |
|---|---|---|---|
| <ul style="list-style-type: none">• Tritium migration• Trapping, diffusion, solubility• Multiple species tracking | <ul style="list-style-type: none">• Heat transfer• Thermal hydraulics• Vapor & aerosol tracking• Reactor accidents | <ul style="list-style-type: none">• HTO modeling• Lithium fire accidents• Multiple working fluids | <ul style="list-style-type: none">• Fully integrated capabilities• Steady-state & transient analysis including accident scenario simulations |
|---|---|---|---|

MELCOR-TMAP



● = developed by Sandia National Laboratory (SNL)

● = developed by Idaho National Laboratory (INL)

TMAP/MOD1 (1988)

Initial release of the Tritium Migration and Permeation (TMAP) code

MELCOR 1.8.2 (1993)

An improvement on previous versions of MELCOR based on Fortran 77 for analysis of light water reactors (LWRs) & related technologies

MELCOR 1.8.6 (2005)

Models for spent fuel pools (SFPs), hydrogen chemistry, flashing, etc. were included in this new release of MELCOR

MELCOR 2.2 (2017)

Improved code architecture based on Fortran 90 including dynamic memory allocation, point kinetics models, turbulent deposition models, etc.

TMAP4 (1992)

Improved version went through extensive verification & validation (V&V) efforts; has a wide distribution & user base

MELCOR for ITER (1994)

Enhanced version of MELCOR 1.8.2 with modeling capabilities to address modeling & safety issues for ITER. Continues to be used for ITER analysis & safety documentation: "Rapport Préliminaire de Sûreté" (Preliminary Report on Safety – RPrS), non-specific site safety reports (NSSR-1 & NSSR-2), & Generic Site Safety Report (GSSR)

MELCOR-TMAP

Includes improvements and modifications made in previous versions of MELCOR for fusion added to 1.8.6

Current version of code in use at INL for analysis of fusion reactors & systems involving tritium transport

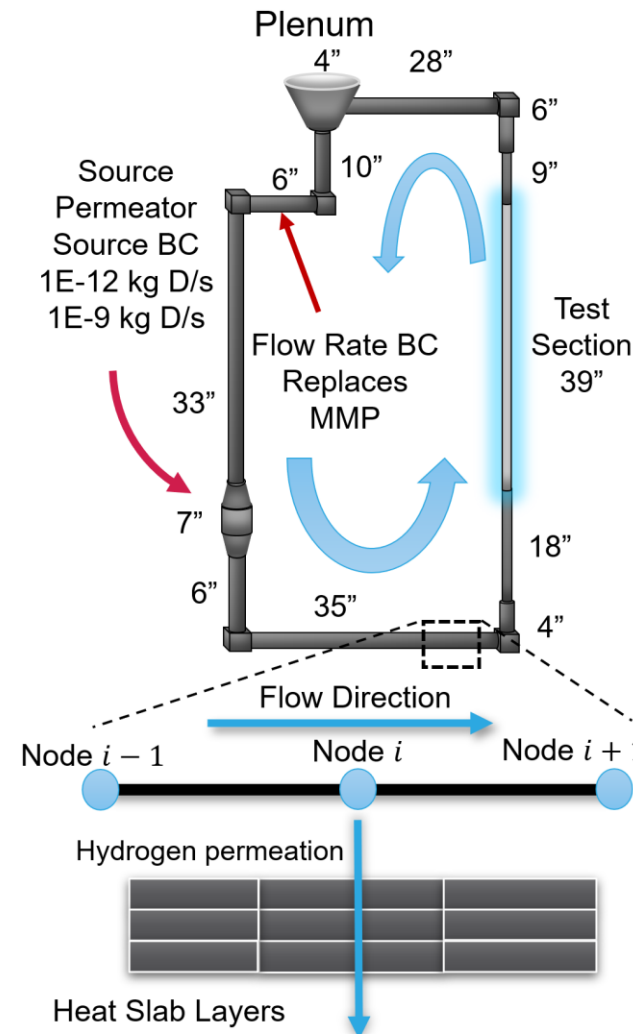
Future Versions of MELCOR-TMAP

Significant software development will be required for integrating MELCOR-TMAP capabilities to the newest version of MELCOR 2.2 in collaboration between INL & SNL

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"

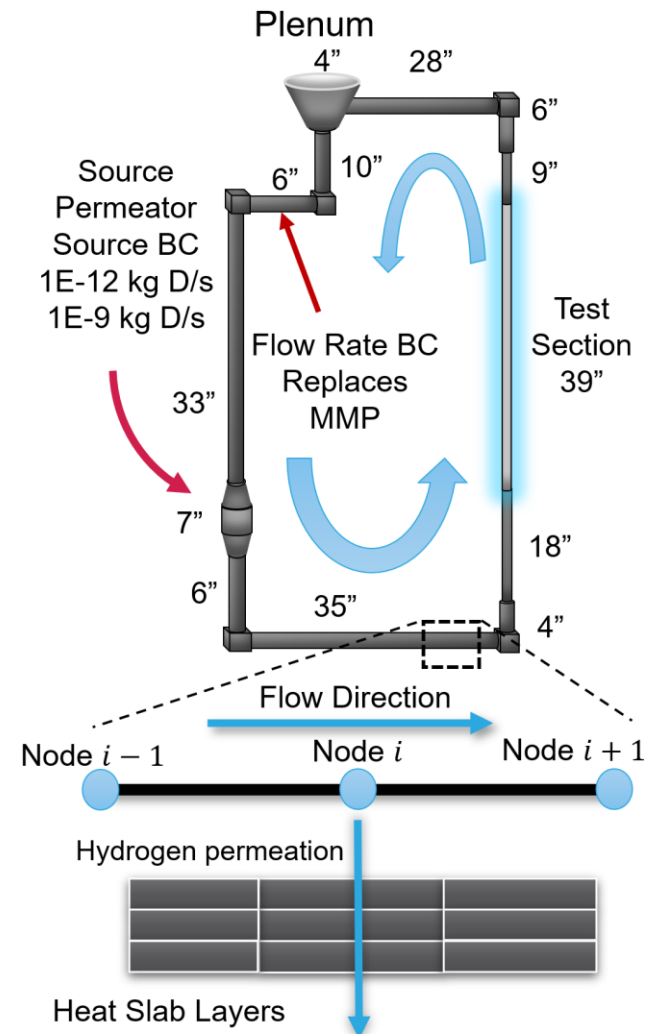
Test Section (Vanadium)

- OD: 0.5"
- ID: 0.46"
- Wall thickness: 0.02"

TEX Model in MELCOR-TMAP



- TEX experiment has been modeled in MELCOR-TMAP using several simplifications and assumptions:
 - Insertion of deuterium at source permeator set as a source term boundary condition (BC)
 - Moving magnet pump (MMP) replaced with a pipe & set as a flow rate BC
 - Volumes immediately outside of test section vacuum (furnace, etc.) are neglected and replaced by BCs and initial conditions (ICs) as appropriate



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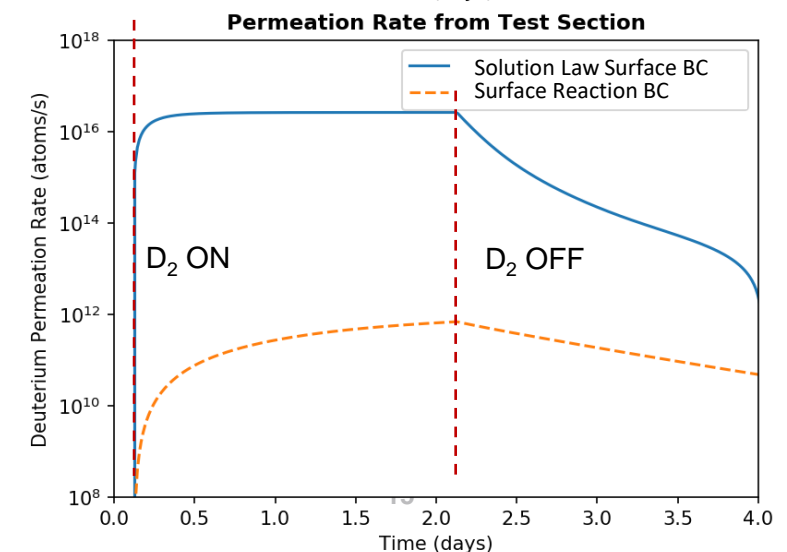
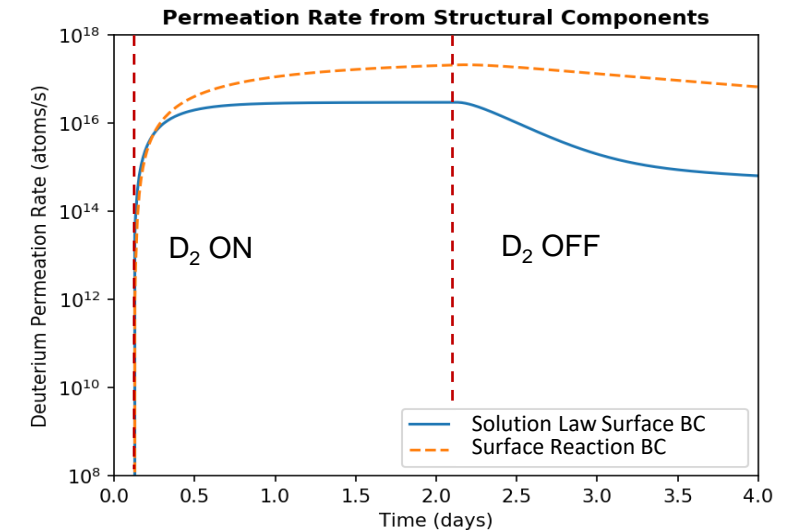
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Test Section (Vanadium)

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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 Simulations

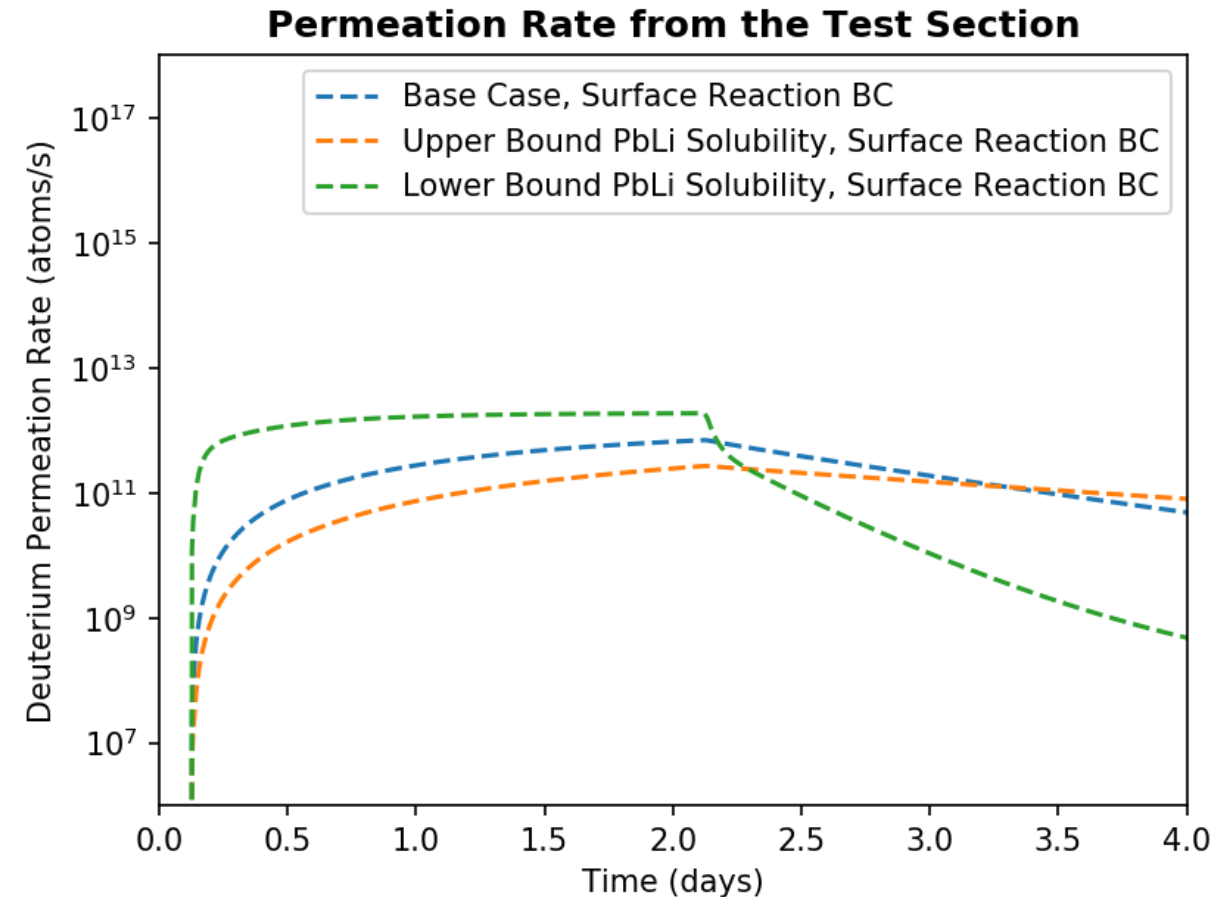


- Sensitivity of permeation rates from test section to multiple parameters was performed in MELCOR-TMAP:
 - PbLi solubility
 - Recombination of permeator material
 - Deuterium source rate

Sensitivity to PbLi Solubility



- PbLi solubility modified:
 - Upper bound¹
 $= 3.6e+22 \text{ atoms}/(\text{m}^3 \cdot \text{Pa}^{1/2})$
 - Nominal case²
 $= 1.4e+23 \cdot \exp(-0.13/kT) \text{ atoms}/(\text{m}^3 \cdot \text{Pa}^{1/2})$
 - Lower bound³
 $= 7.7e+20 \cdot \exp(-0.01/kT) \text{ atoms}/(\text{m}^3 \cdot \text{Pa}^{1/2})$
- 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.

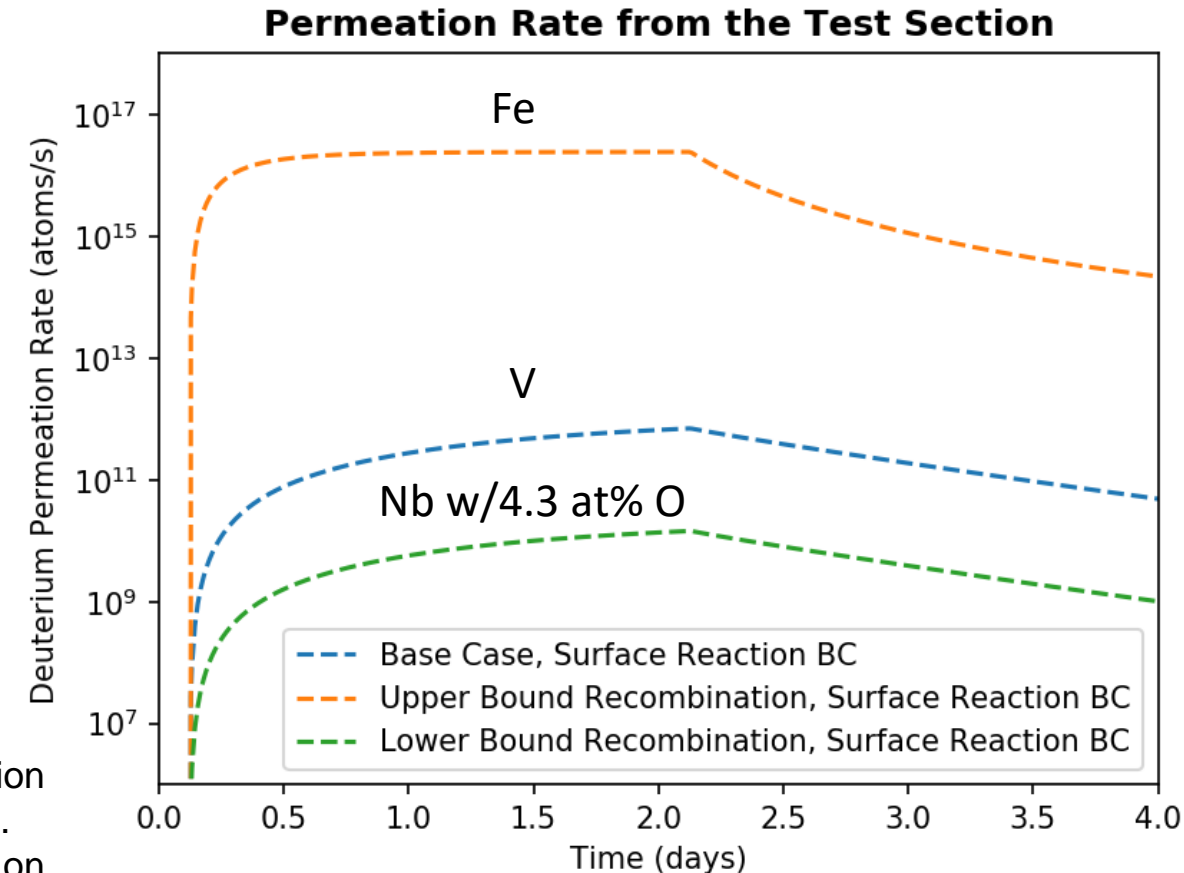
²A. Aiello, Ciampichetti A., and Benamati G. 2006. "Determination of hydrogen solubility in lead lithium using sole device." Fusion Eng. Des. 81, no. 1: 639-644

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

Sensitivity to 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.

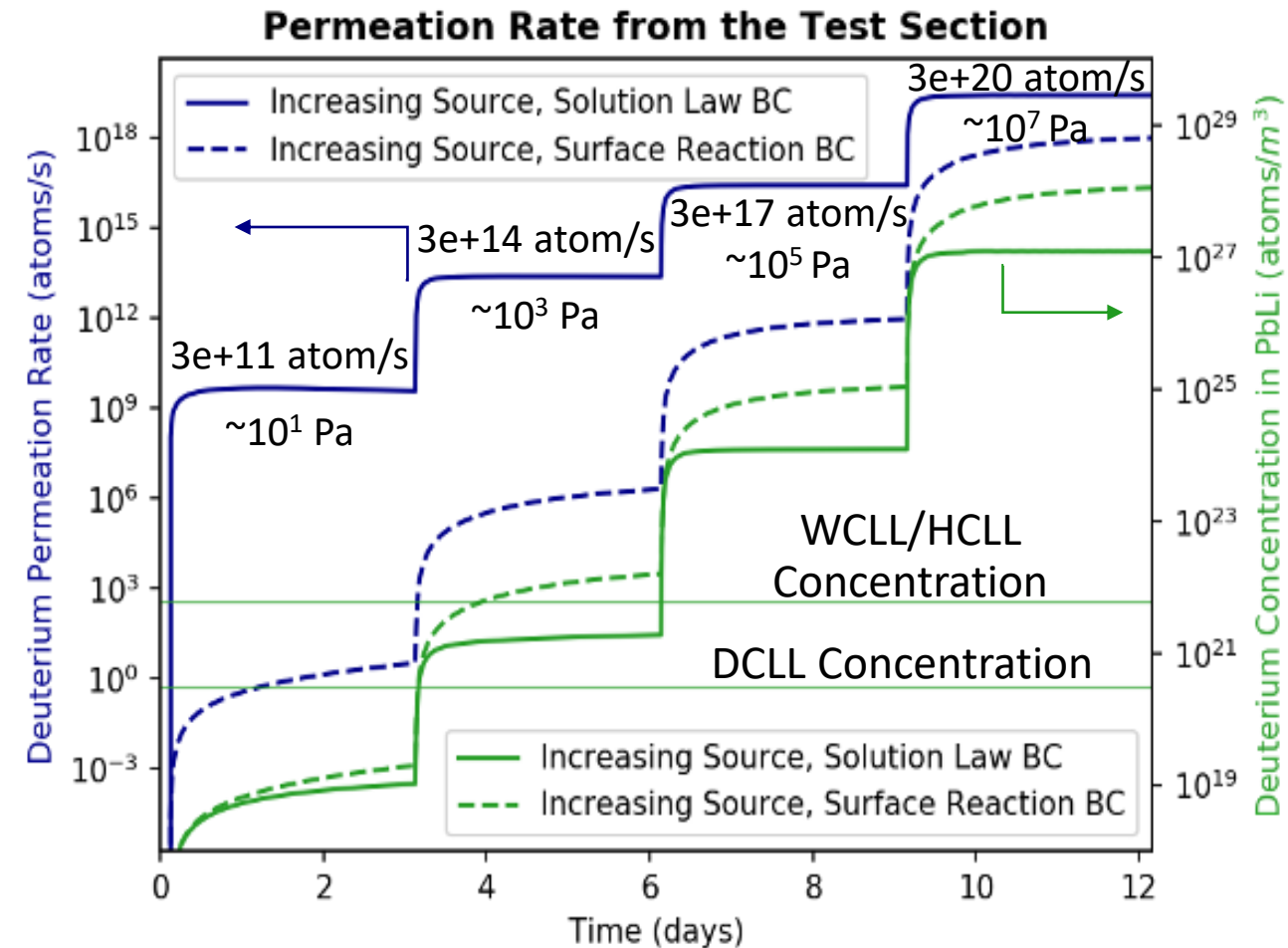
²T. Fuerst, P.W. Humrickhouse, C.N. Taylor, M. Shimada. 2021. "Surface effects on deuterium permeation through vanadium membranes." J. Membrane Sci. 620:118949

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 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)



Summary of Sensitivity Simulations



- Simulations show permeation rate from test section are less sensitive to range of PbLi solubilities & highly sensitive to permeator recombination and source rates

Conclusions



- TEX is designed to test the effectiveness and various component designs for a vacuum permeator extraction system
- Modeling of TEX using MELCOR-TMAP provides insights into dependence of hydrogen permeation based on material properties & other operation parameters
- Continued testing & modeling of system parameters will provide further understanding of extraction efficiency & safety of TEX for operation using tritium

Future Work



- Incorporate Pd coating & interdiffusion barriers into MELCOR-TMAP model
 - Pd coating intended to enhance recombination coefficient at permeator surface to greatly increase H permeation rates
 - Focus of ARPA-E GAMOW project with Colorado School of Mines
- Include MELCOR-TMAP model for transfer of hydrogen from PbLi in the plenum to the vapor phase



Questions?

