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FESTIM
FINITE ELEMENT SIMULATION OF TRITIUM IN MATERIALS

Validation of FESTIM Hydrogen Transport Modeling in FLiBe Through HYPERION Permeation Data

Huihua Yang, James Dark, Abhishek Saraswat, Weiyue Zhou, Kevin Woller, Eathan Peterson, Remi Delaporte-Mathurin

Plasma Science and Fusion Center, MIT, USA

Email: huihuay@mit.edu

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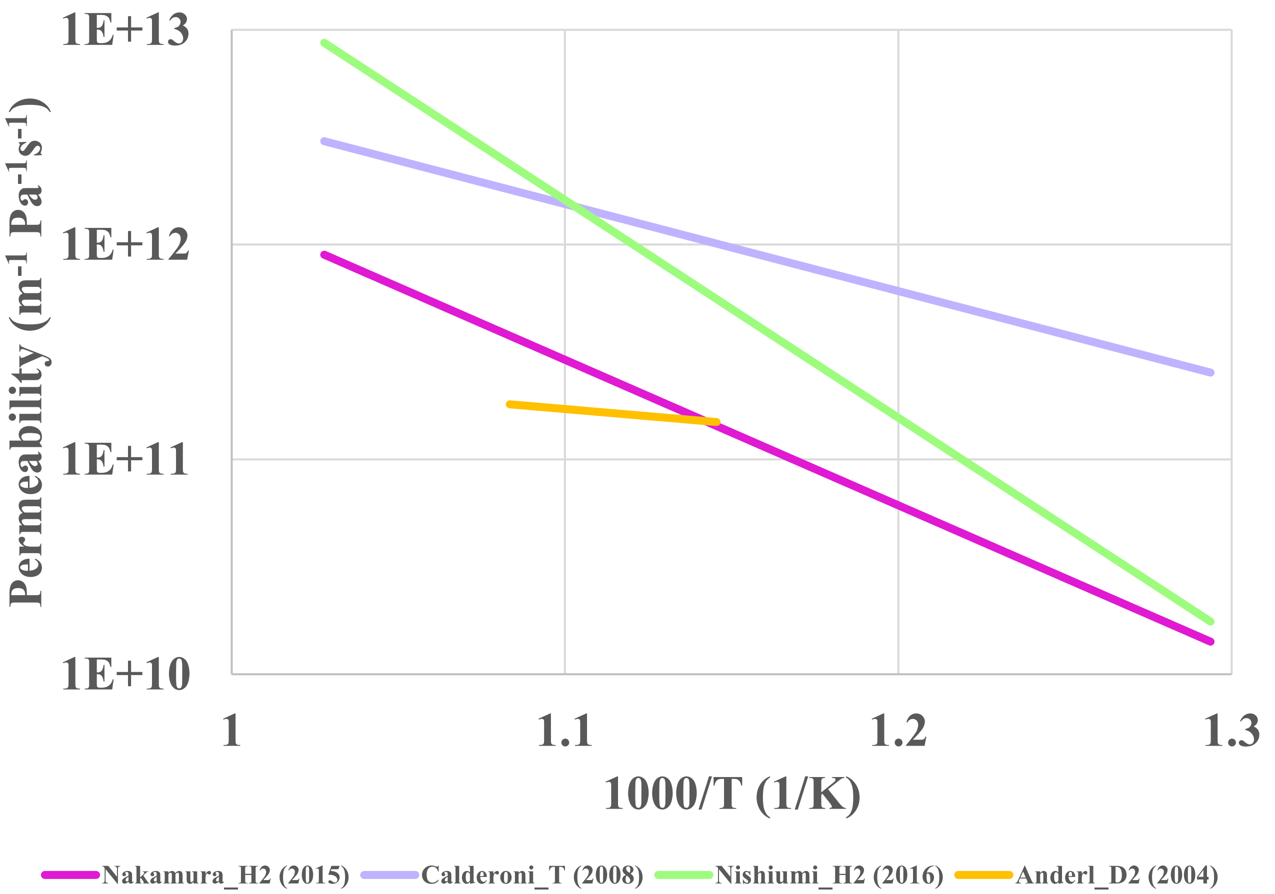
Background & Motivation

- FLiBe is a leading molten salt candidate for liquid blankets (MIT LIBRA Project → ARC)
- Tritium control in liquid blankets design requires accurate hydrogen transport models and transport data
- Existing FLiBe permeability data are **scarce & inconsistent**
- Traditional 1D model neglect leakage paths → permeability errors up to order(s) of magnitude



biased permeability leads to **incorrect tritium inventory predictions**

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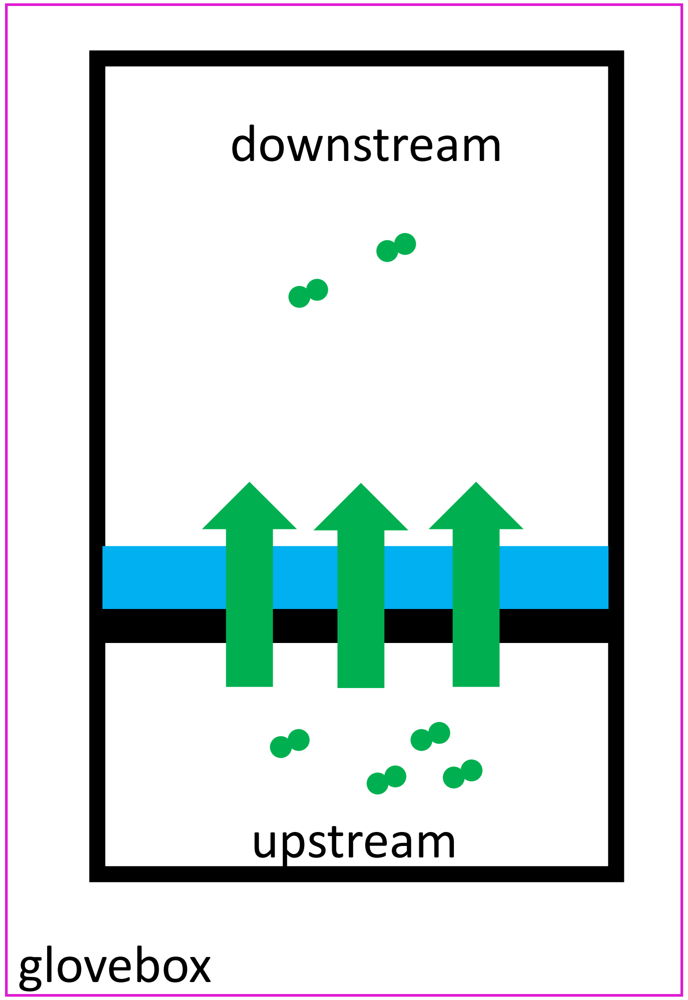
Background & Motivation

Goal:

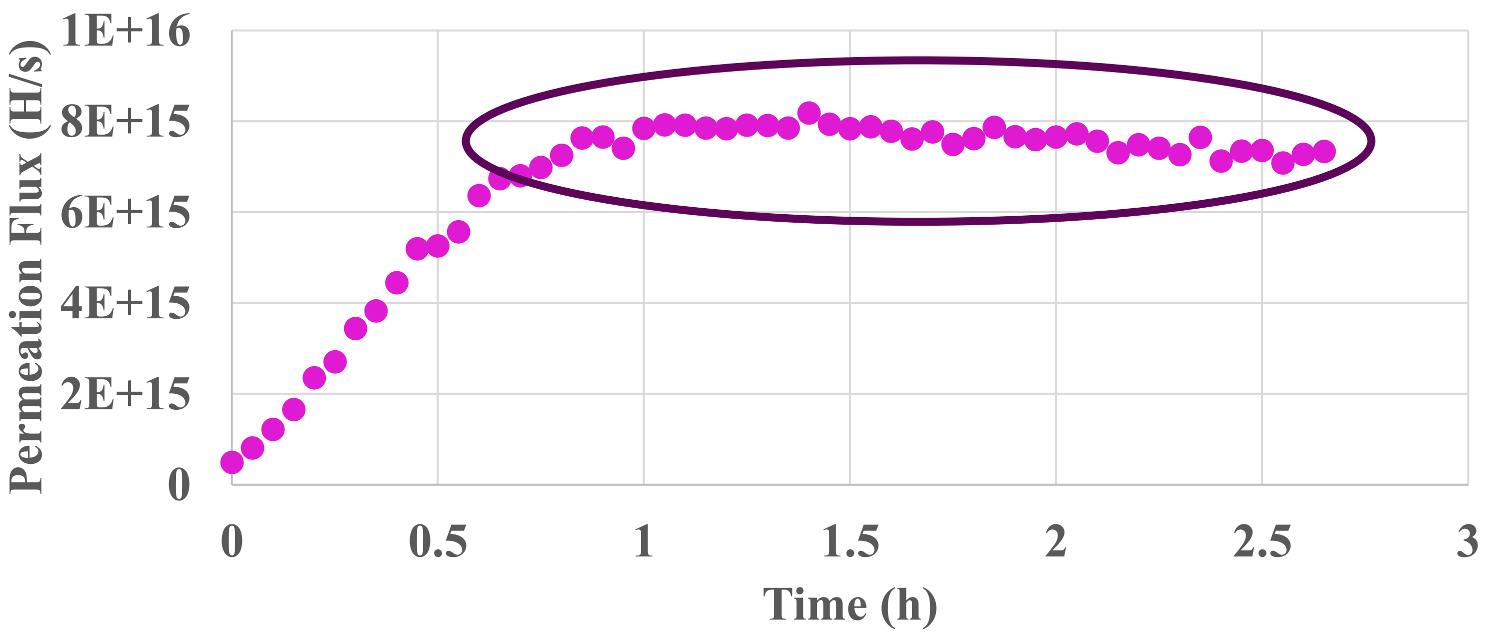
Apply FESTIM to interpret MIT's HYPERION (hydrogen permeation) experiments, accounting for **2D hydrogen transport** and **realistic leakage boundary conditions**, to **extract FLiBe permeability** for liquid blanket design

- **First integrated simulation-experiment framework** for molten-salt permeation, enabling geometry-resolved permeability extraction
- **First direct assessment of sidewall leakage effects** in molten-salt permeation experiment
- Demonstration that **1D models bias permeability** estimations
- **A consistent workflow** to derive Arrhenius-form H-isotope permeability across different materials

HYdrogen PERmeatION (HYPERION) Experiment



- Impose partial pressure of H2 upstream
- H permeates through the Ni membrane and FLiBe liquid **+ Ni vessel**
- Measure the desorption flux of H downstream
- Repeat at different temperatures



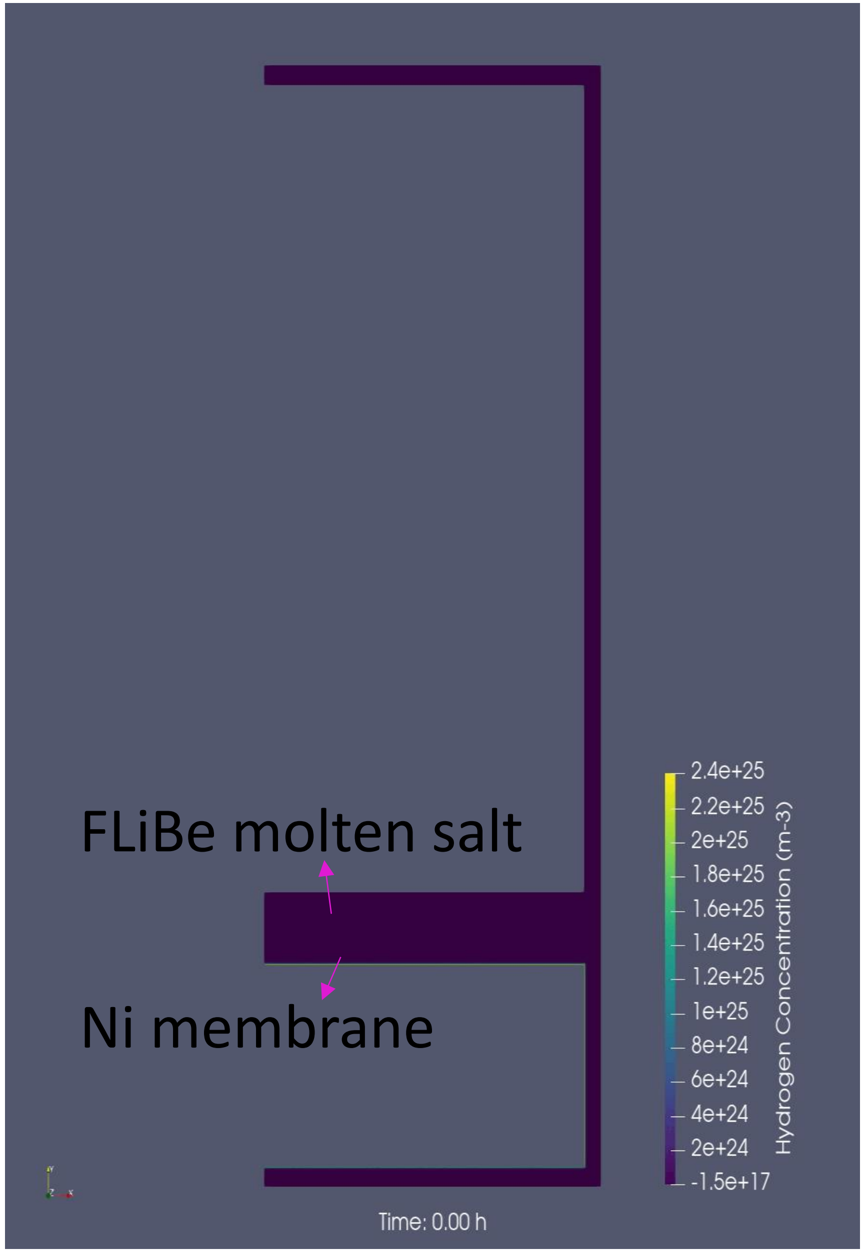
Quasi-2D geometry → sidewall becomes an important flux path

FESTIM (Finite-Element Simulation of Tritium in Materials)

- Multi-dimension, multi-species (H isotopes) transport
  - Diffusion
  - Trapping and de-trapping
  - Decay
  - Isotope exchange
- Multi-region chemical potential continuities
  - Metal-liquid, metal-metal interfaces
- Heat transfer
- Advection
- **Open-source**

2D FESTIM model for HYPERION experiment

- 2D axisymmetric
- H diffusion in Ni membrane + molten FLiBe + Ni vessel
- Potential continuity across the metal-liquid interface
- Sidewall leakage: boundary conditions
- Outputs: spatial hydrogen concentration
- Flux extraction: $J = -D\nabla c$



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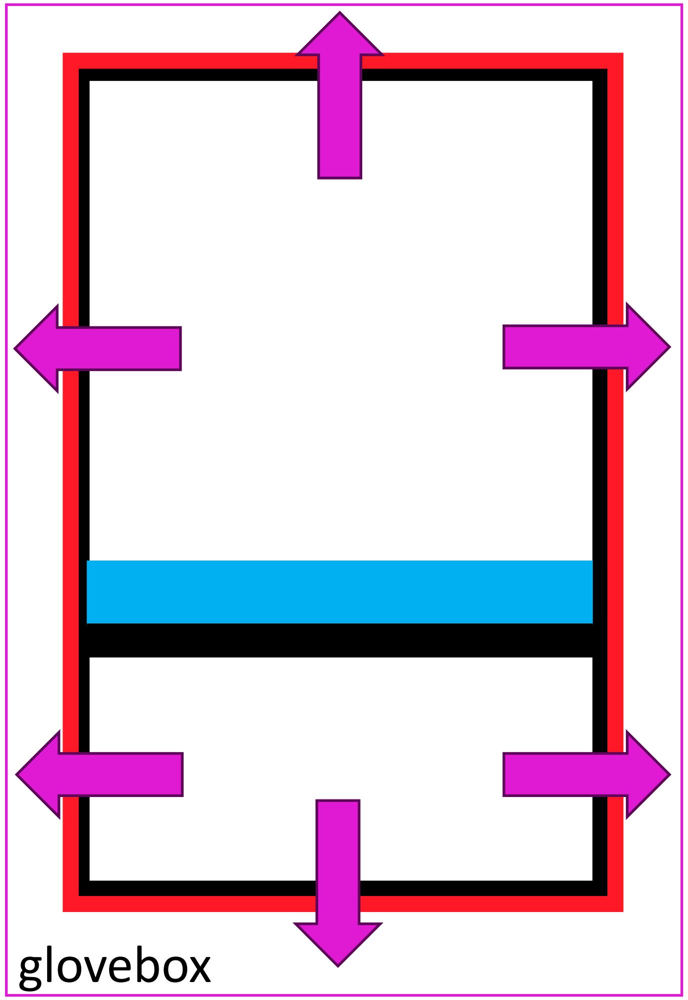
Boundary conditions



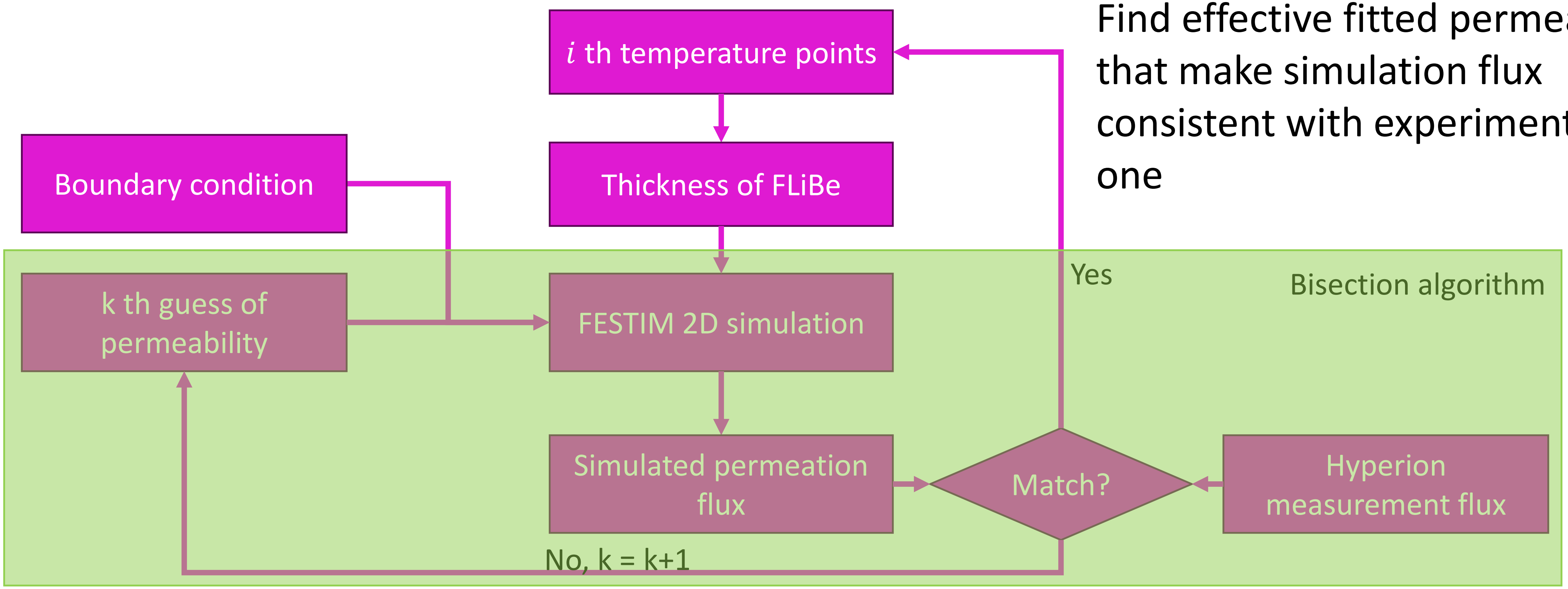
Two extreme cases

- Ideal coating → sealed vessel → no H leakage to glovebox
  - Basic assumption used in traditional 1D interpretation
- No coating → full leakage → H free release to the glovebox

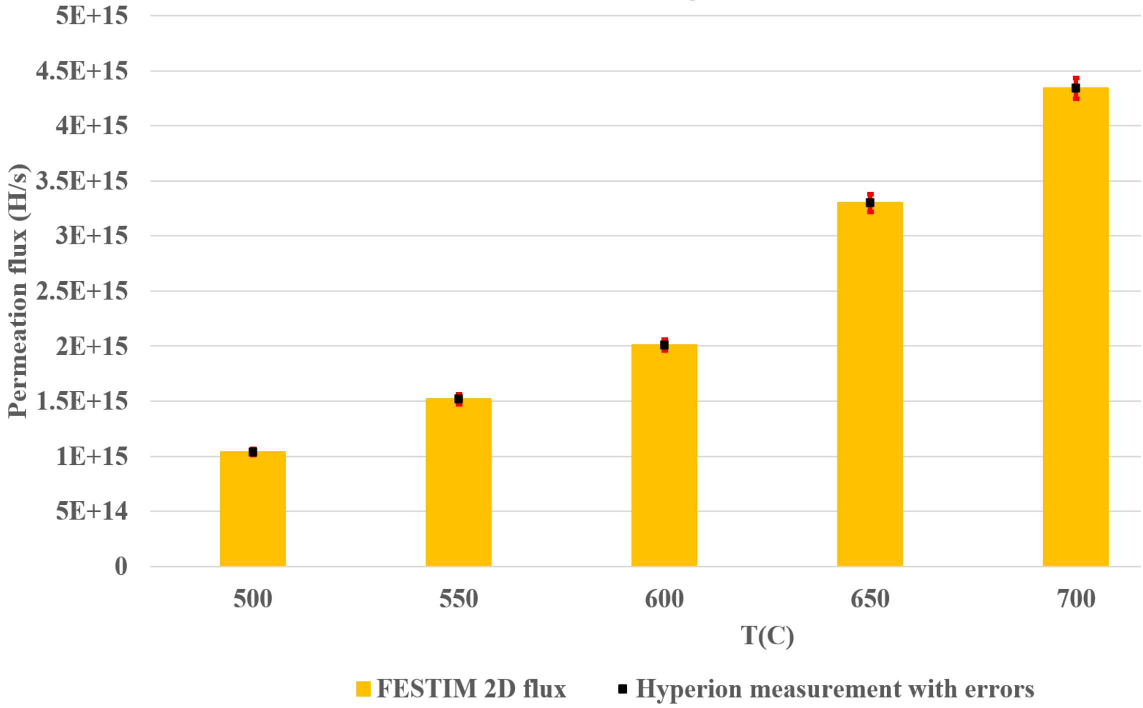
- Real experiment (partial coating) lies between these limits

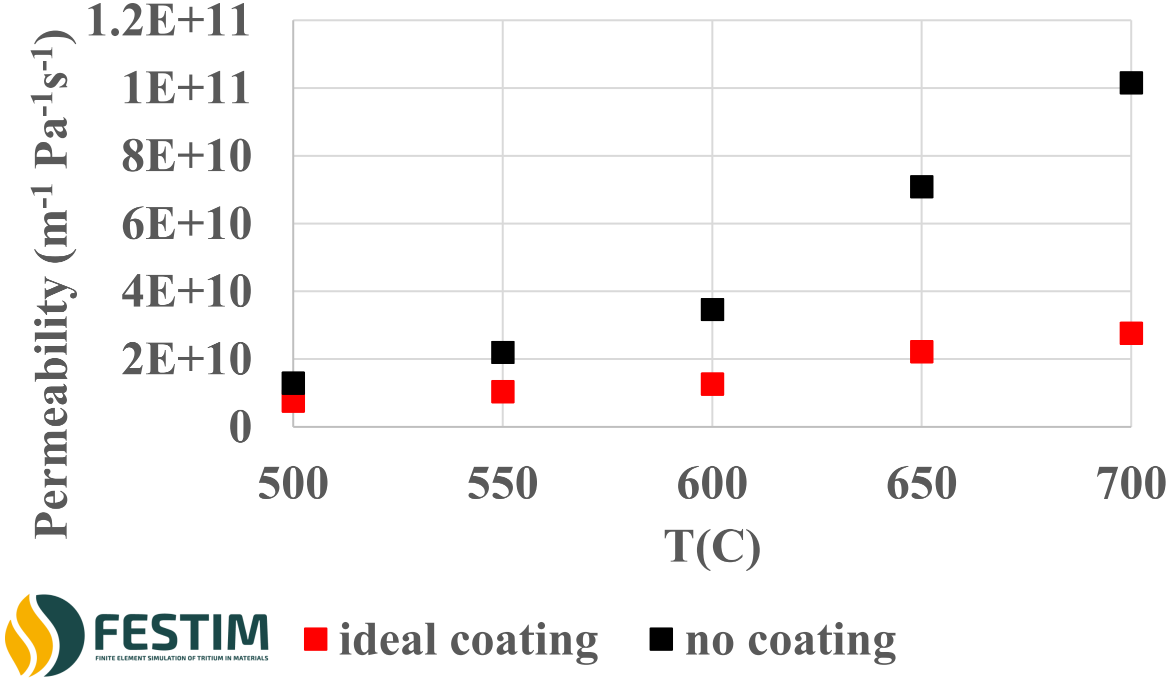
FESTIM-Hyperion Workflow

Temperature → Compute salt thickness → Setup BC → Guess **permeability** → Run 2D FESTIM → Compared to experiment → **Bisection update**



Find effective fitted permeability that make simulation flux consistent with experimental one





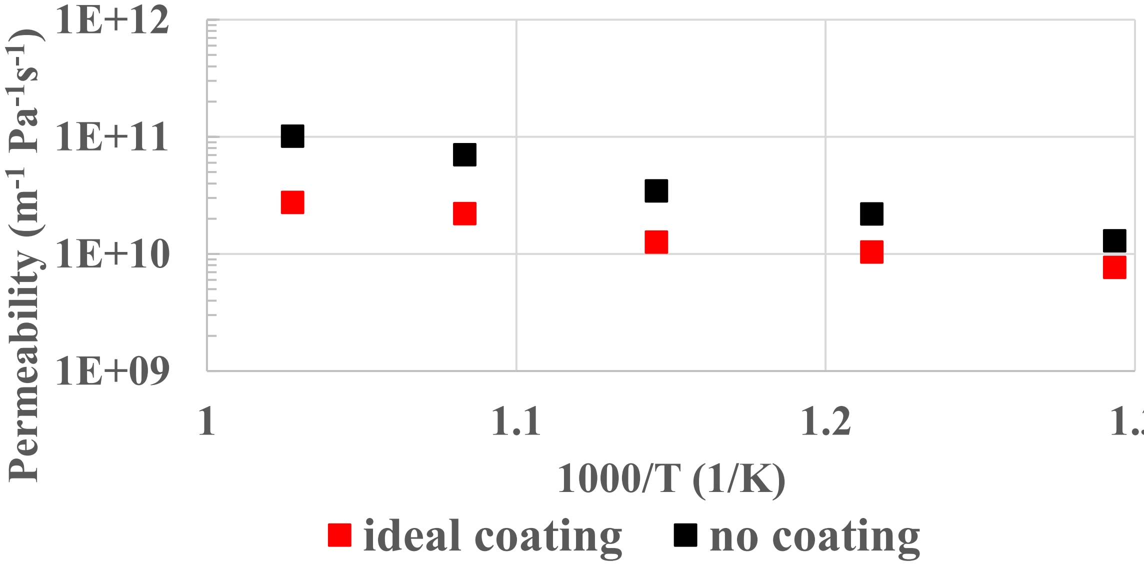
Permeability properties can be expressed as Arrhenius format:

$$P = P_0 \exp\left(-\frac{E_P}{k_B T}\right)$$

$$\ln P = \ln P_0 - \frac{E_P}{k_B T}$$

Weighted linear fitting, $w_i = \frac{1}{\sigma^2_{\ln P_i}}$, with

$\ln P_i$ relevant measurement uncertainty



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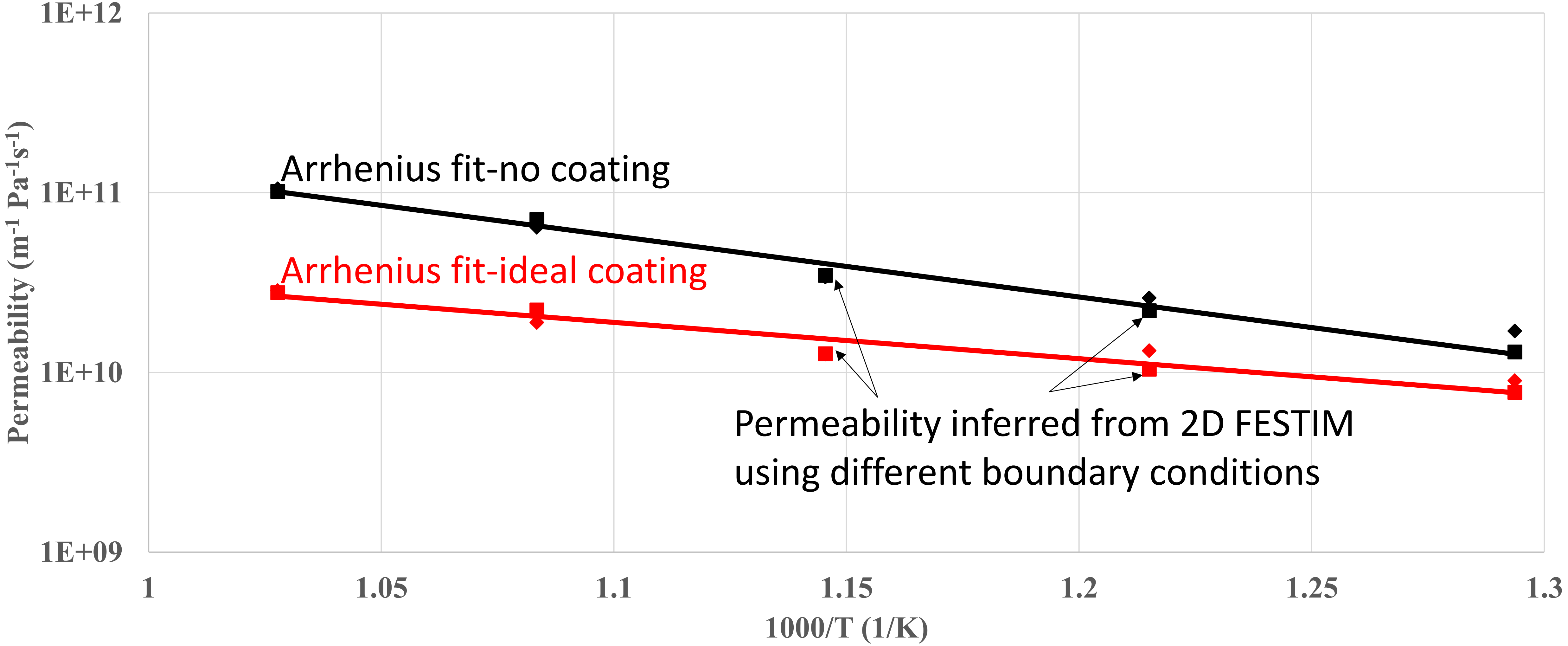
Fitting permeability



FLiBe permeability lies between $3.17 \times 10^{12} \exp\left(-\frac{0.401}{k_B T}\right) \sim 3.16 \times 10^{14} \exp\left(-\frac{0.675}{k_B T}\right)$

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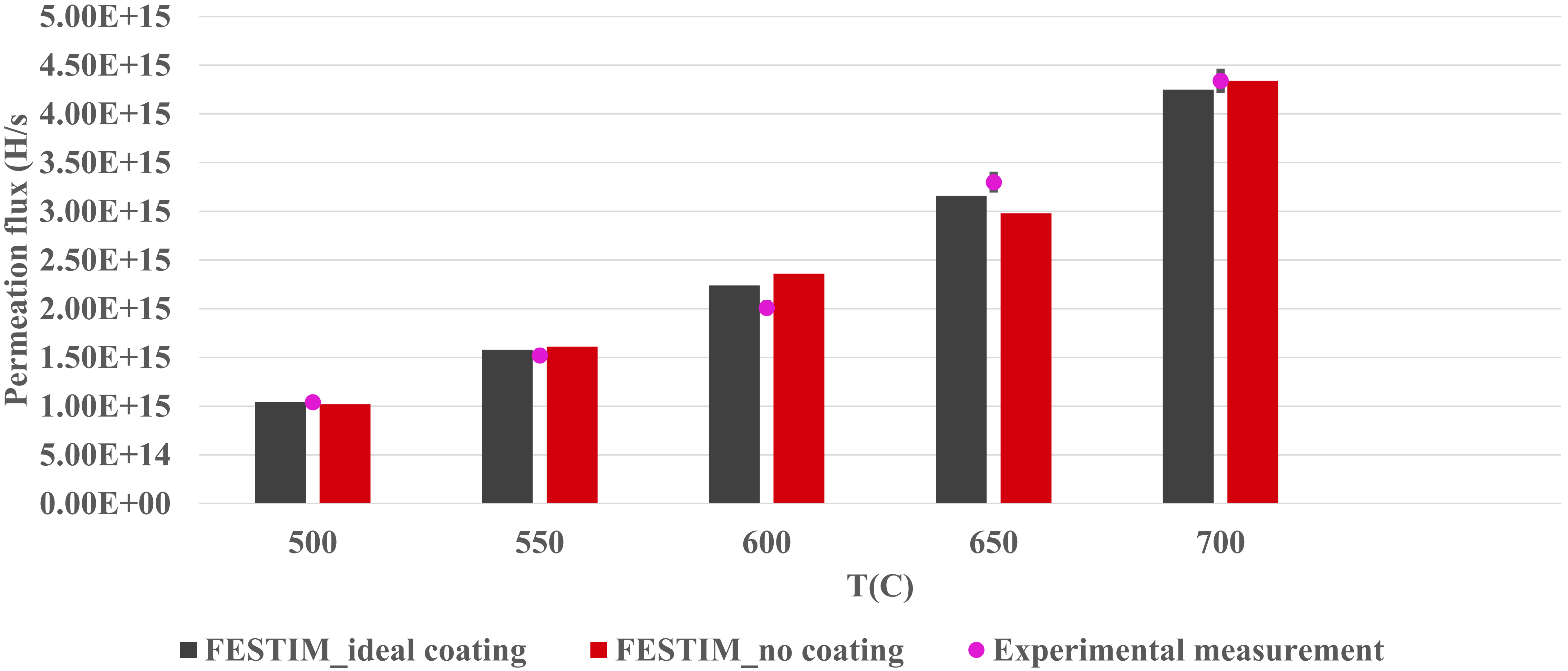
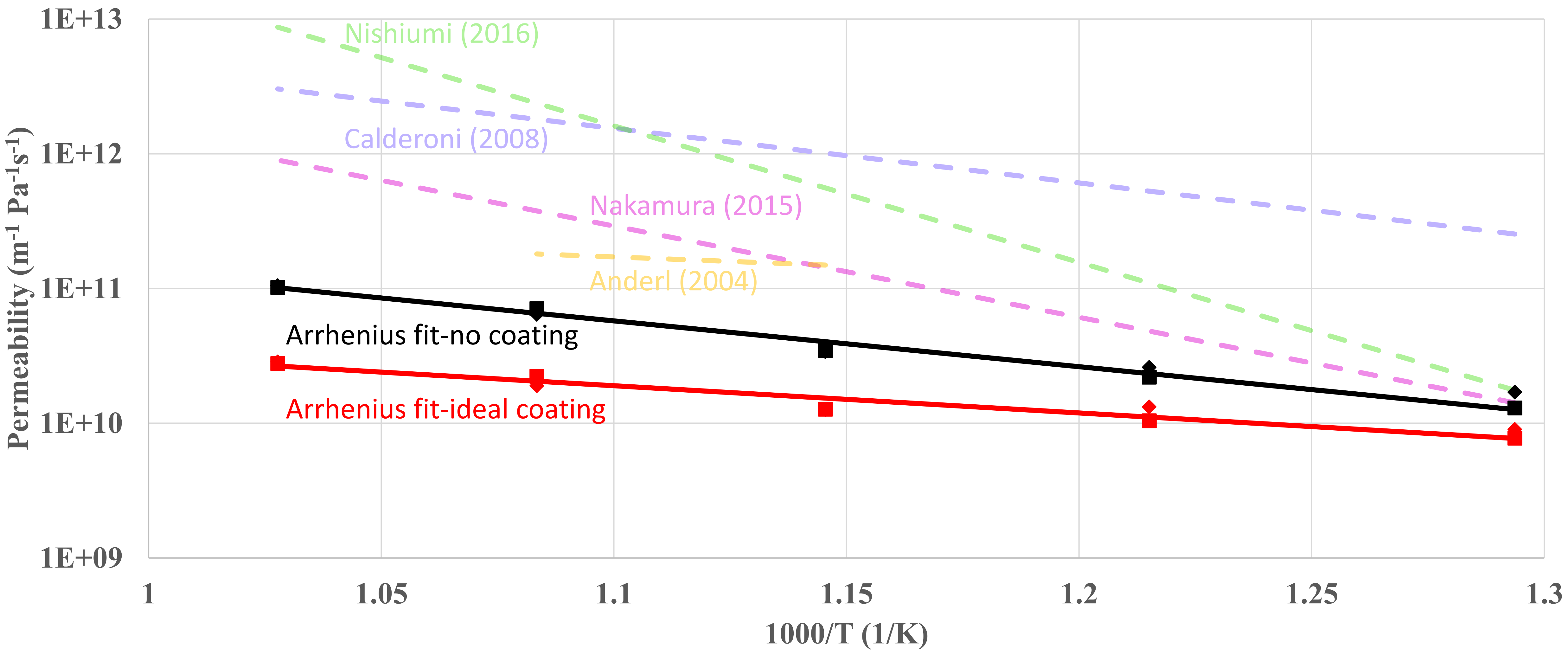
Fitting performance



- Simulation match experiment
- Different inferred permeability, similar fluxes, **ONLY due to boundary condition choice**

Fitting permeability



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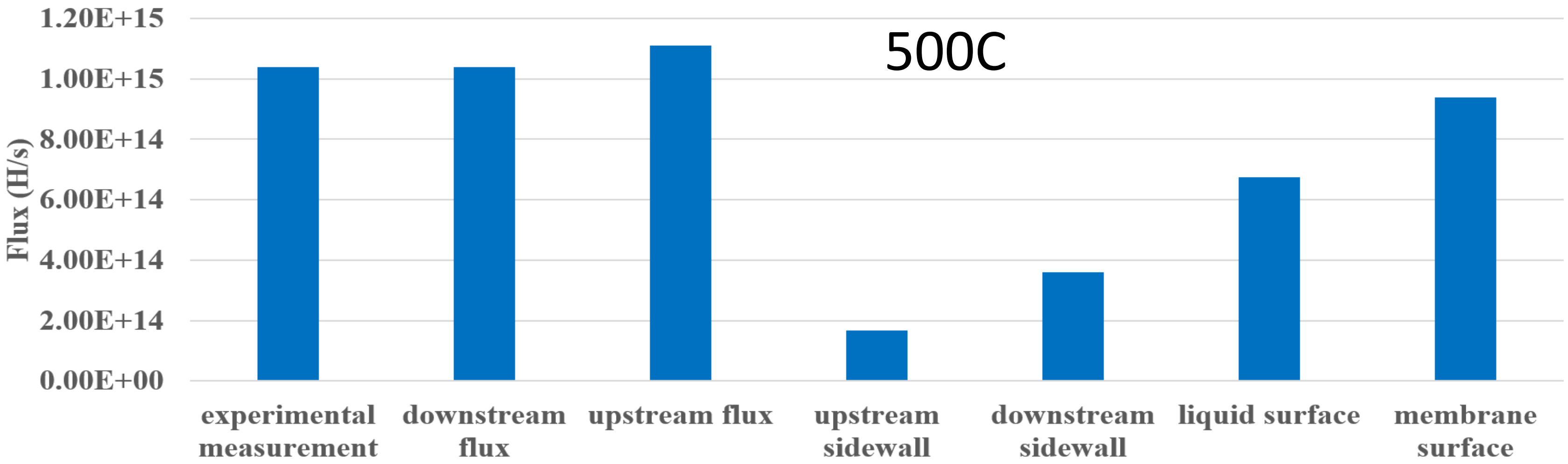
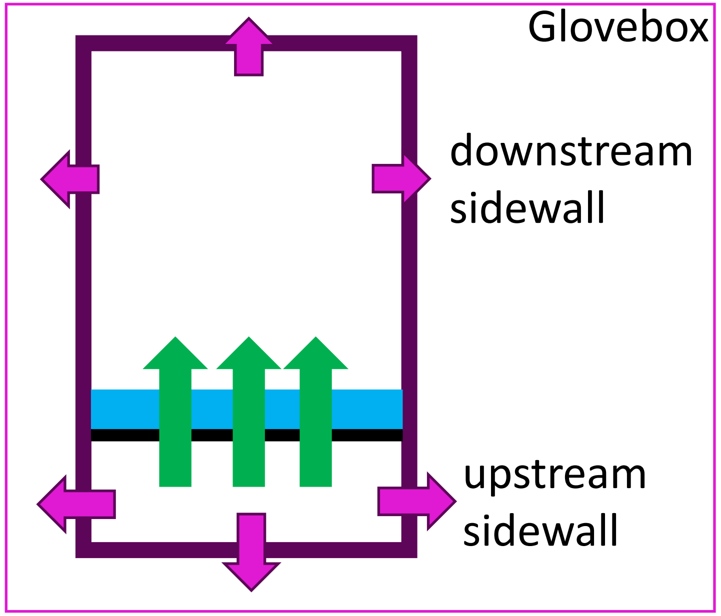
Hydrogen permeation behavior investigation





500-700C

Case	Upstream sidewall share Relative to upstream flux	Downstream sidewall share Relative to downstream flux
Ideal coating	15% - 21%	35% - 53%
No coating	~94%	13% - 61%

Sidewall transport contribution increases with temperature

Geometric effects are non-negligible, should be modeled explicitly

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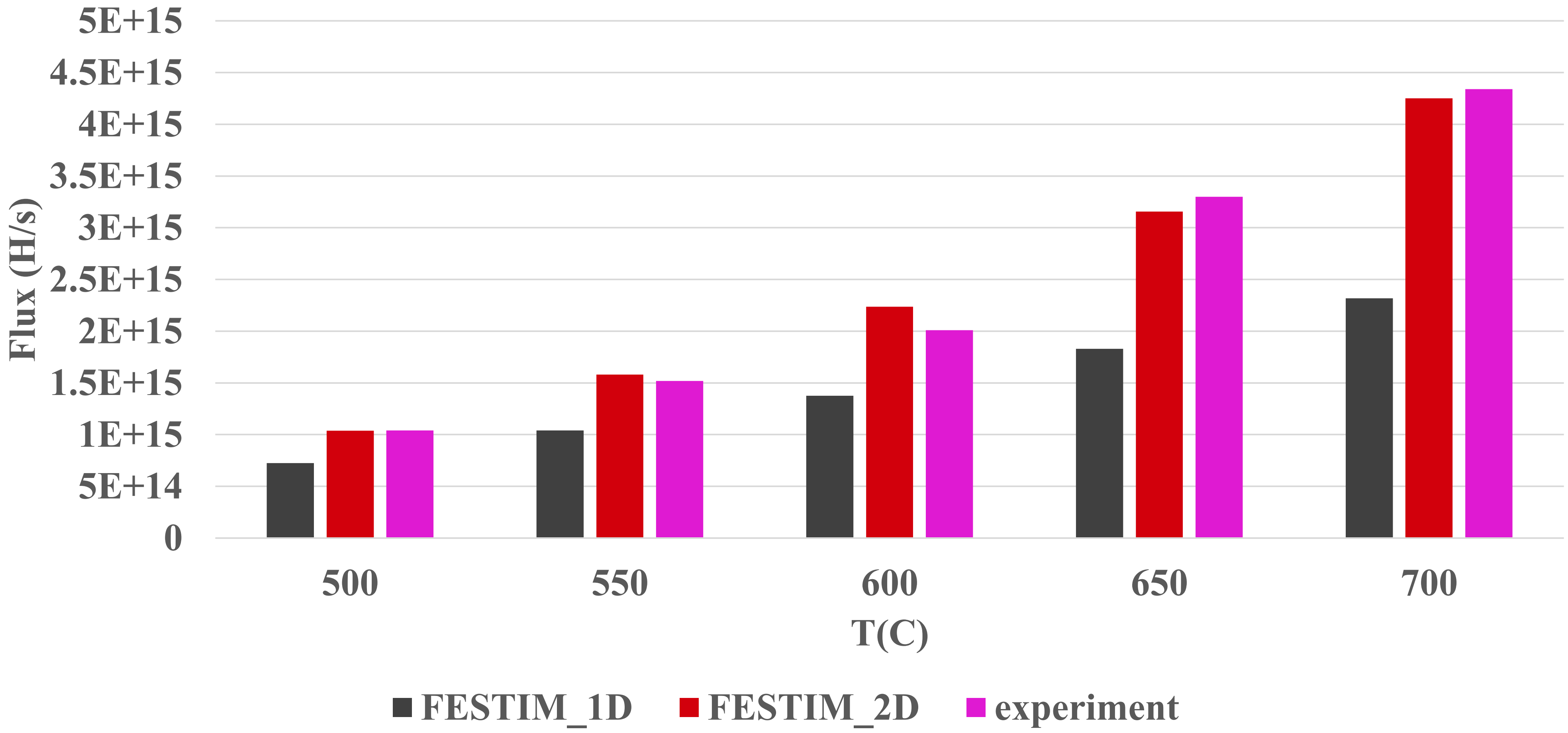
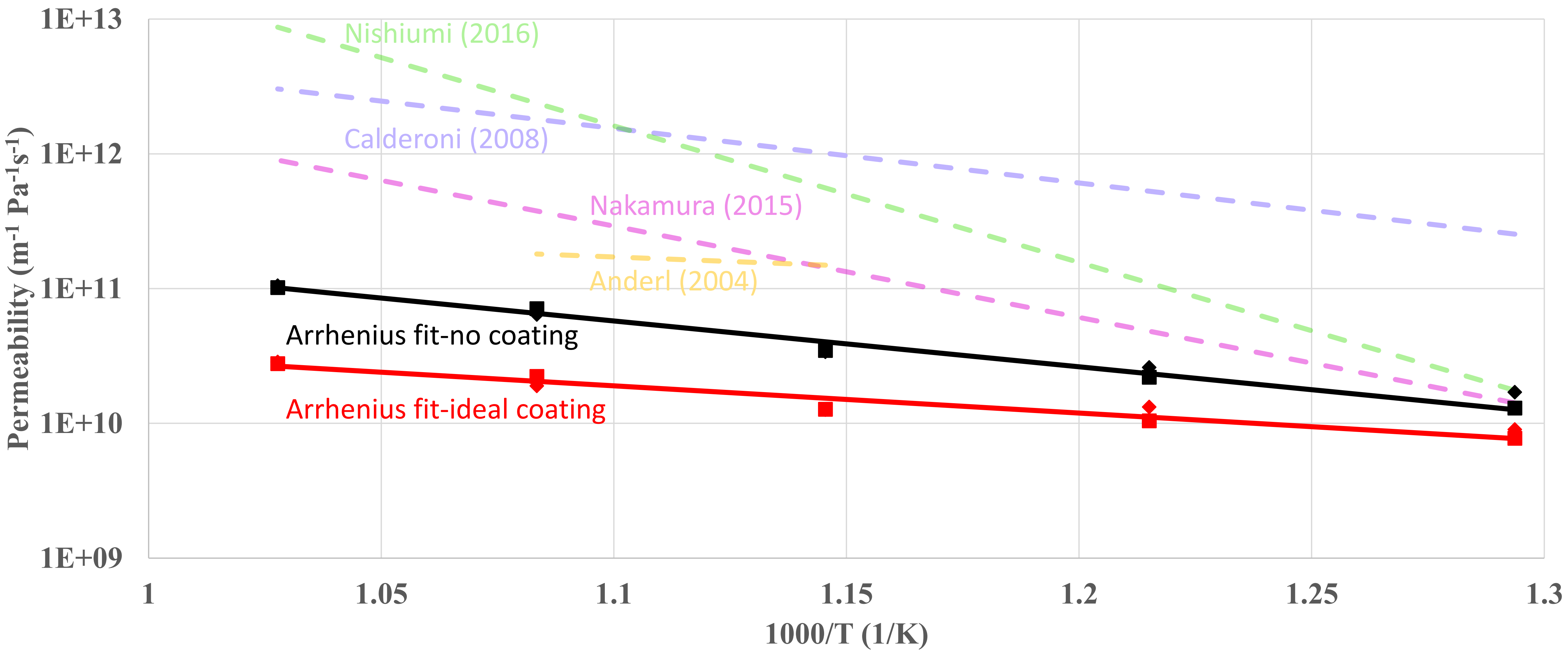
1D vs 2D simulation result comparisons



- 1D models **underestimate** flux (~ 50% at 700C) → forces all H permeate through the shortest path and ignores real leakage geometry
- Extracted permeability from 1D is **artificially high**, especially at high temperature

Fitting permeability



FLiBe permeability lies between $3.17 \times 10^{12} \exp\left(-\frac{0.401}{k_B T}\right) \sim 3.16 \times 10^{14} \exp\left(-\frac{0.675}{k_B T}\right)$

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Conclusions & Takeaways

- Geometry strongly biases inferred FLiBe permeability
  - Neglecting sidewall leakage in 1D models leads to systematic **overestimation of permeability**, with the error growing at high temperature

- **First 2D, coating-condition-aware interpretation** of molten-salt permeation experiment using FESTIM

$$3.17 \times 10^{12} \exp\left(-\frac{0.401}{k_B T}\right) \sim 3.16 \times 10^{14} \exp\left(-\frac{0.675}{k_B T}\right)$$

- Direct impact on **tritium inventory & safety margins**

- **A transferable digital-twin framework** for permeation analysis
  - Applicable across molten salts, structural metals, and permeation test configurations

Future direction

- **Interfacial bubble formation** has been observed at the metal-FLiBe interface, modifying the effective hydrogen permeability

- This introduces a **three-phase coupled transport problem**: solid-liquid-gas

- **Next step**: develop and integrate a **bubble nucleation, growth, and retention model** into FESTIM

- Swap configuration experimental data will be used to **quantify and interpret** the bubble-induced transport effects

Acknowledgement

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- Experimental support
  - Abhishek Saraswat and Dr. Weiyue Zhou for conducting Hyperion permeation experiment

- Modeling & code development
  - FESTIM development team

- Collaborations
  - LIBRA project collaboration

More details: Huihua Yang @ huihuay@mit.edu

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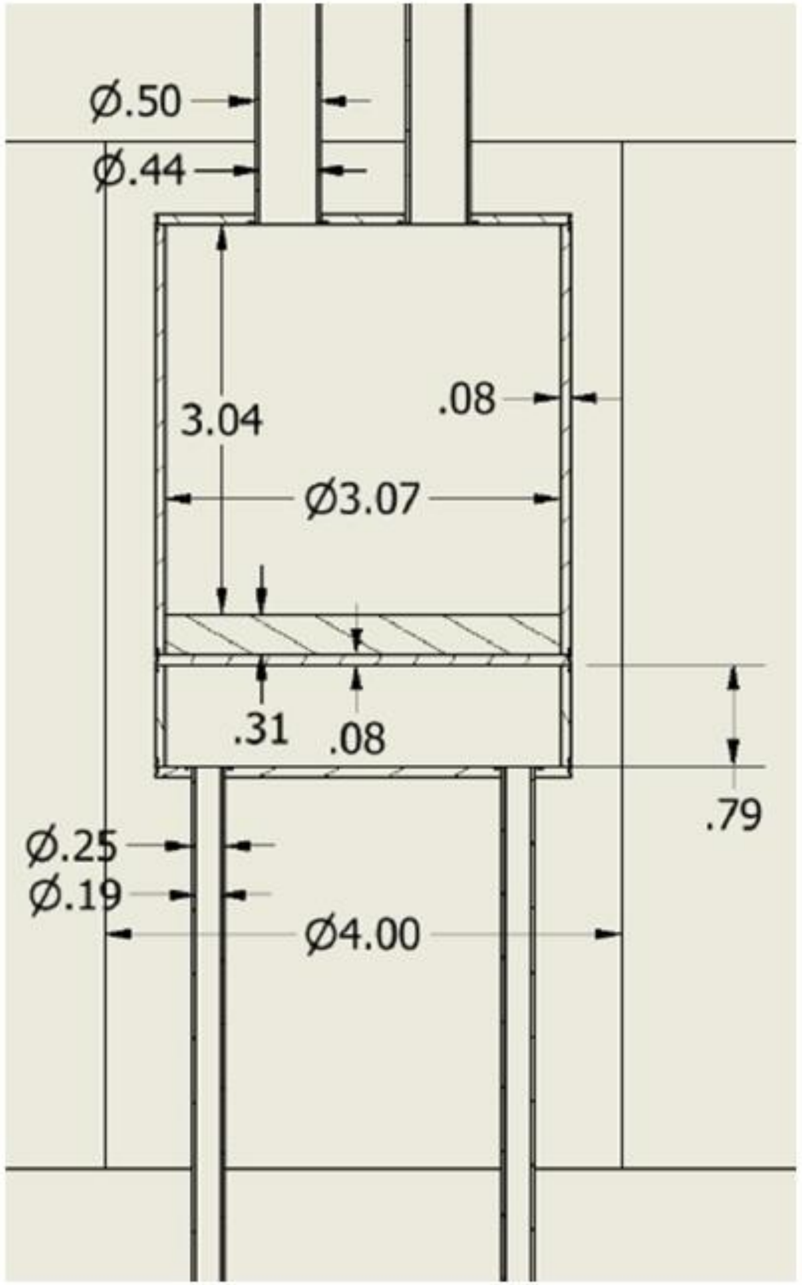


Unit: inches

Key parameters

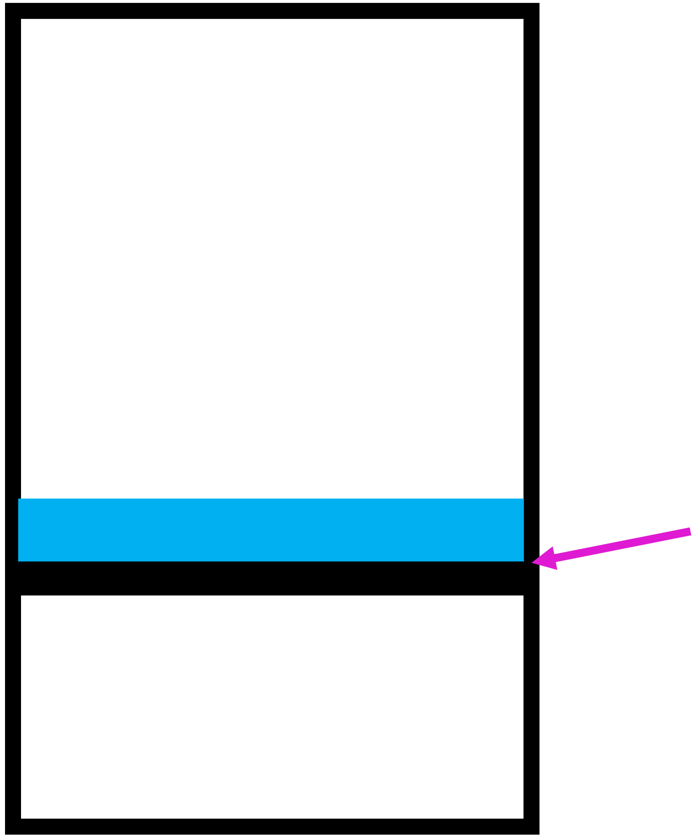
- Ni membrane: 0.002 m
- FLiBe thickness:

Salt layer thickness	m
Thickness @ 500C	0.005139858
Thickness @ 550C	0.005194021
Thickness @ 600C	0.005249337
Thickness @ 650C	0.005305845
Thickness @ 700C	0.005363582

- Repeat the measurement, each temperature repeat twice
- T=500-700C

Experimental condition

- Normal: P_upstream ~ 1e5 Pa, P_down: 5-20Pa



$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c)$$

$$\left(\frac{c_{Ni}}{K_{s,Ni}}\right)^2 = \frac{c_{FLiBe}}{K_{H,FLiBe}}$$

$$J = -D \nabla c$$

Uncertainty

- Mesh uncertainty almost negligible, mesh independence study has done

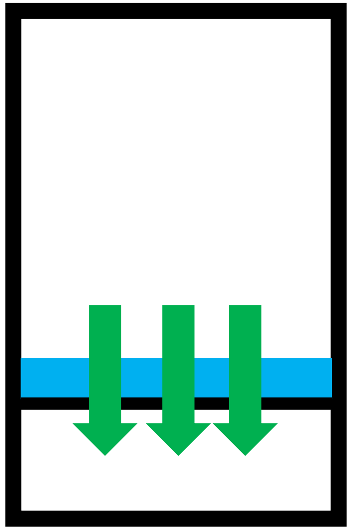
- Relative system error from gas chromatograph (GC): $u_s = \frac{\Delta \mathrm{PPM_{GC}}}{\mathrm{PPM_{GC}}} \approx 1.00011\%$

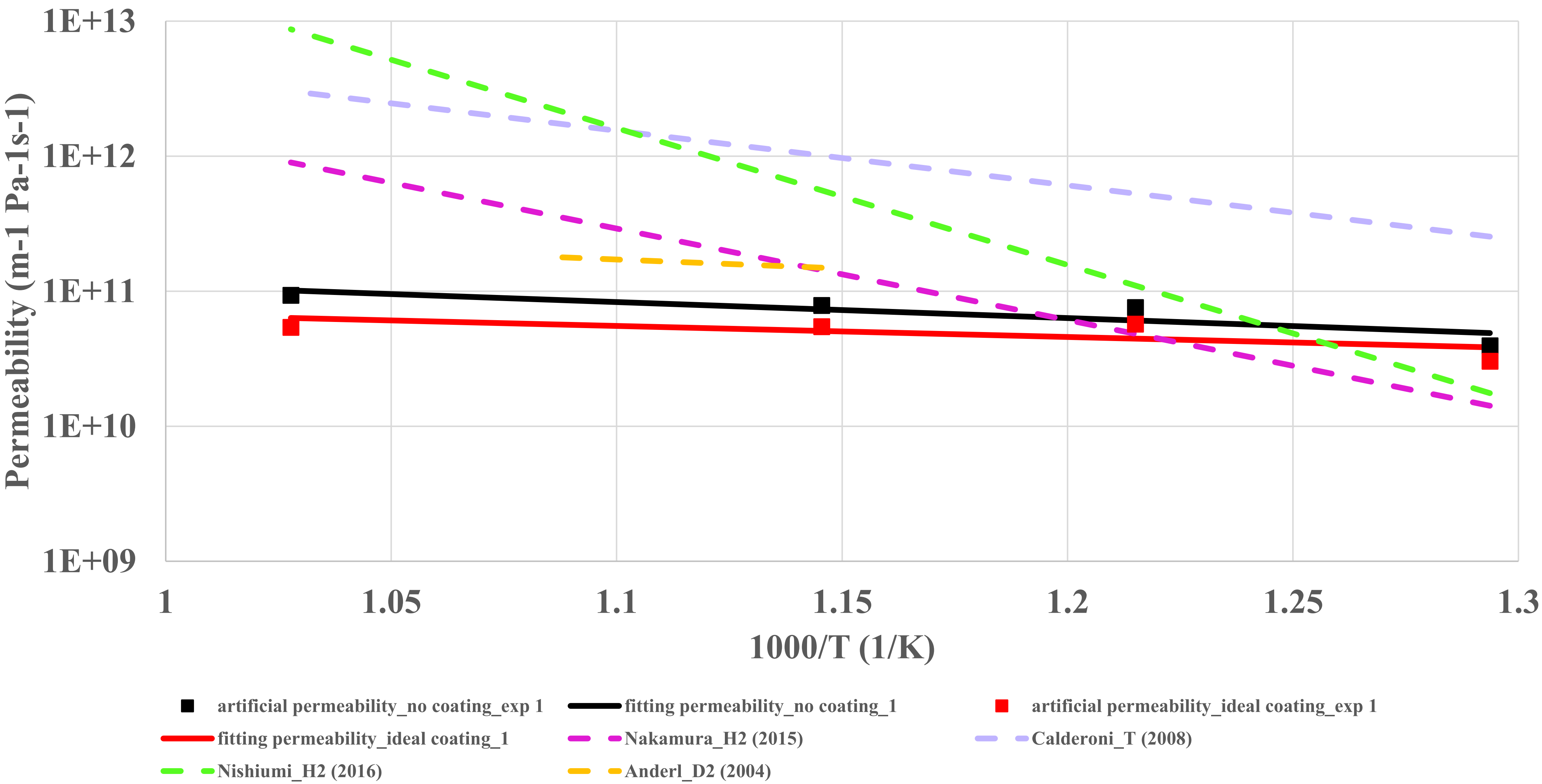
- Measurement error u_r:
  - N steady state measurement data $y_i, i = 1 \ldots N$
  - Average: $\bar{y}$
  - Standard deviation: $std = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \bar{y})^2}{N-1}}$
  - Standard uncertainty of the mean: $u_r = \frac{std}{\sqrt{N}}$

- Combined standard uncertainty $u_c = \sqrt{(u_s \bar{y})^2 + u_r^2}$

- Expanded uncertainty at 95% confidence: U = 2 u_c

Fitting of permeability: swap configuration liquid side as upstream





$$4.38 \times 10^{11} \exp\left(-\frac{0.162}{k_B T}\right) \sim 1.67 \times 10^{12} \exp\left(-\frac{0.235}{k_B T}\right)$$

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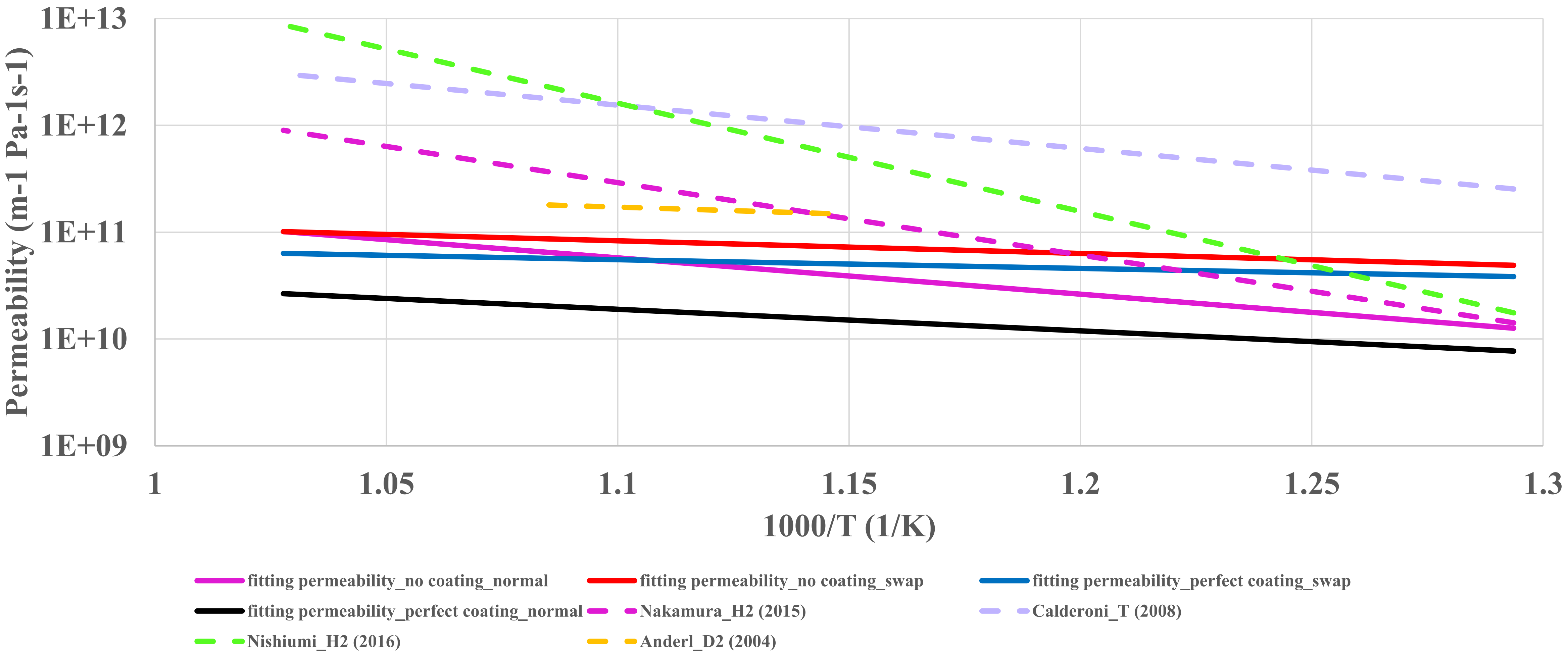
Fitting of permeability



FLiBe details

LiF–BeF_2 molten salt (typically 66–34 mol%)
Originally developed at ORNL (MSRE)

- Excellent Neutron Performance
  - Lithium enables efficient tritium breeding
  - Beryllium acts as a neutron multiplier
  - Supports compact, high-performance blanket designs
- High Thermal Stability
  - Operating range: ~500–900 C
  - Low vapor pressure → compatible with near-vacuum systems
  - Excellent heat transfer capabilities
- Chemical & Radiological Stability
  - Low swelling under irradiation
  - No violent boiling under off-normal conditions
  - Chemically stable fluoride system
- Liquid Blanket = Self-Healing & Reconfigurable
  - No radiation damage accumulation like solid blankets
  - Salt can be purified, reprocessed, and reused online

Property	**FLiBe (LiF–BeF_2)**	**FLiNaK (LiF–NaF–KF)**	**PbLi (Liquid Metal)**
Tritium breeding	✓	✓	✓
Neutron multiplier	✓	✗	✓
Phase	Molten salt	Molten salt	Liquid metal
Operating temp.	~500–900 C	~450–900 C	~500–800 C
Vapor pressure	Very low	Very low	Very low
Electrical conductivity	Low (good for MHD)	Low	High (severe MHD issues)
Chemical safety	Stable fluorides	Stable fluorides	Reactive with air/water
Radiation damage	Self-healing (liquid)	Self-healing	Self-healing
Tritium leakage risk	Moderate–High	Low–Moderate	High
Data availability	Sparse & inconsistent	Moderate	Extensive