INL/CON-22-67575-Revision-0

Calibration of a mesoscale tritium transport model for ceramic breeder materials in TMAP8 using experimental data

June 2022

Changing the World's Energy Future

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Idaho National Laboratory

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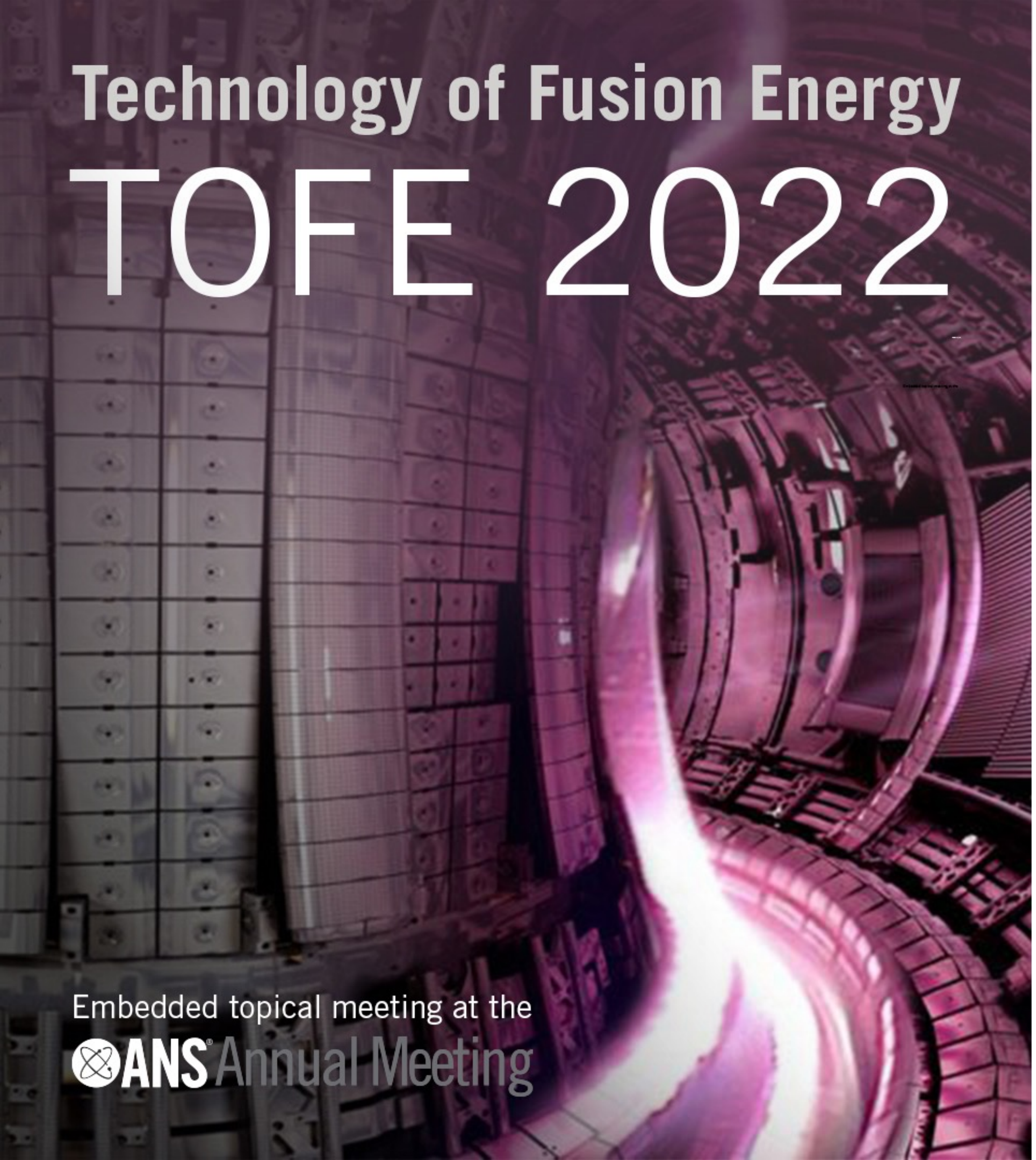

Calibration of a Mesoscale Tritium Transport Model for Ceramic Breeder Materials in TMAP8 Using Experimental Data

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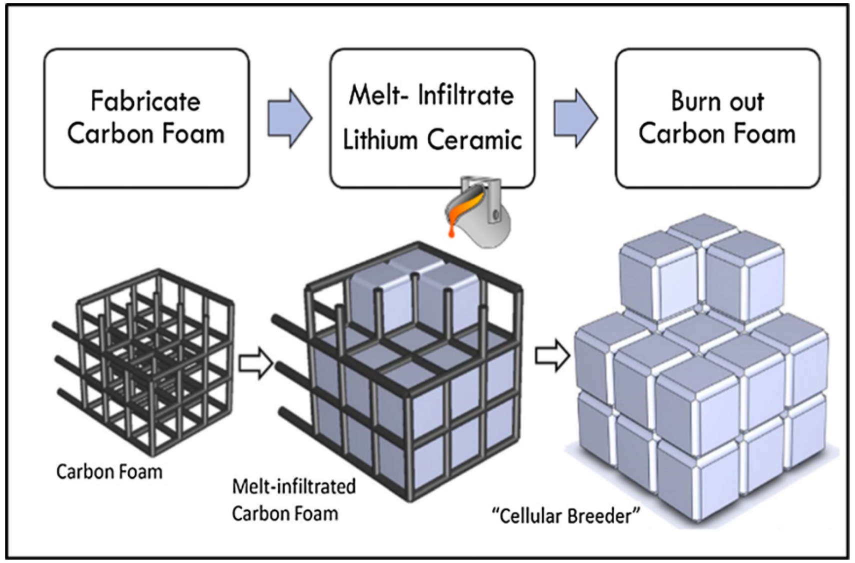
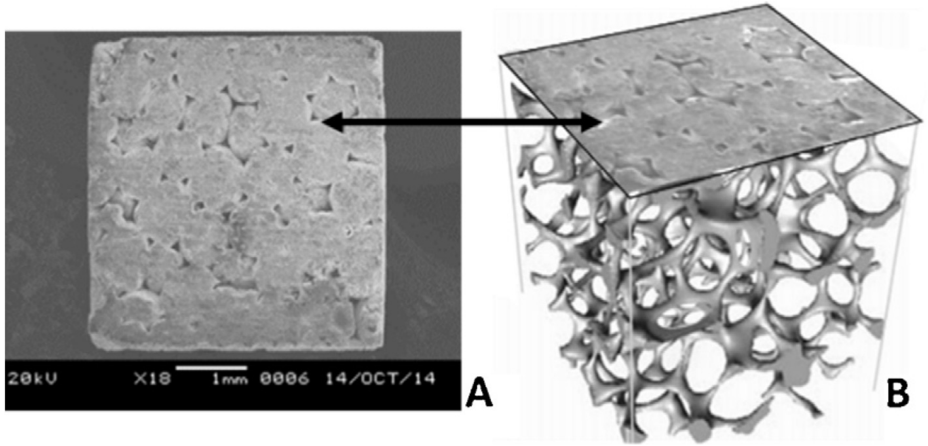
Outline

- Background on tritium transport and cellular ceramic breeder (CCB) materials
- Tritium transport modeling at the pore scale using TMAP8
- Model calibration and sensitivity study
- Enabling 2D and 3D simulations in real CCB pore structures
- Conclusions and future work

Tritium Transport and Cellular Ceramic Breeder (CCB)

- The blanket must breed tritium at the same rate or faster than it is consumed (Tritium Breeding Ratio = TBR > 1)
- CCB materials as a potentially transformative blanket concept





- High density
- High pore interconnectivity
- Hopes for high TBR

Sharafat et al, Fusion Engineering and Design, 2016, vol. 109-111, pp. 119–127

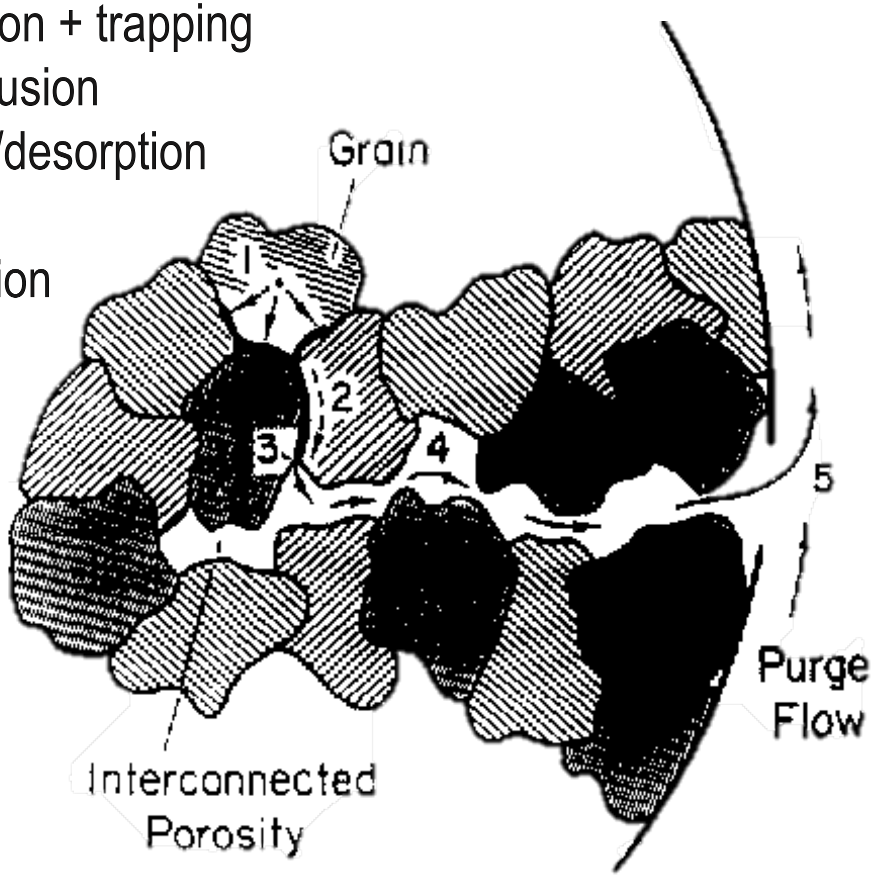
Tritium Transport Modeling at the Pore Scale in TMAP8

- TMAP8 is a MOOSE (Multiphysics Object-Oriented Simulation Environment) derived application
  - Open source and freely available
  - Access to all the physics/features already implemented and verified in MOOSE
  - 1D, 2D, or 3D simulations without extensive additional coding
  - Massively parallel computation
- Unique custom syntax makes it more usable for transport
- New numerical tool to model fusion systems

Tritium Transport Modeling at the Pore Scale in TMAP8

<u>Mechanisms of Tritium Transport:</u>

0. Tritium generation in bulk
1. Intragranular diffusion + trapping
2. Grain boundary diffusion
3. Surface absorption/desorption
4. Pore diffusion
5. Purge flow convection



Different species in the model:

CERAMIC Unlimited Oxygen

Free tritium (T_s) Trapped tritium (T_t)
Free hydrogen (H_s) Trapped hydrogen (H_t)

$$\frac{dX_s}{dt} = \nabla \cdot (D_c \nabla X_s) + \dot{q} - \frac{dX_t}{dt} + 2(K_{gs} - K_{sg})$$

$$\frac{dX_t}{dt} = K_t X_s (X_t^0 - X_t) - K_d X_t$$

SURFACE
Chemical reactions of recombination and attachment at the surface, e.g.,

$$2T_s \rightarrow T_2(g) \qquad K_{sg} = k_{sg}[T_s]^2$$

$$T_2(g) \rightarrow 2T_s \qquad K_{gs} = k_{gs}[T_2](1-\theta)^2, \text{ with } \theta = \frac{[T_s]+[T_t]}{\theta^0 [T_t]^0}$$

PORE

Purge gas (H_2, H_2O)
Gaseous tritium (T_2, T_2O, HT, HTO)

$$\frac{dX_g}{dt} = \nabla \cdot \left(D_p \nabla X_g\right) + (K_{sg} - K_{gs})$$

Federici et al., Journal of Nuclear Materials, pp. 185–213, 173 (1990).

Model Calibration and Sensitivity Study

The aim of the current study is to calibrate the model using quantitative experimental measurements and understand the model's behavior

Model Parameter	Minimum Value	Maximum Value
D_c (μm^2·s^{-1})	10^3	10^8
D_p (μm^2·s^{-1})	10^6	10^{11}
K_D (s^{-1})	10^{-2}	10^2
K_T (s^{-1}·mol^{-1})	10^{16}	10^{20}
$[T_t]^0$ (mol·μm^{-3})	10^{-21}	10^{-15}
θ^0 (-)	1	10^3
k_{sg} (μm^3·s^{-1}·mol^{-1})	10^{13}	10^{19}
k_{gs} (s^{-1})	10^{-2}	10^4

. Select parameter values (Dakota)
. Run simulation (TMAP8/MOOSE)
. Analyze results and compare against experimental measurements using the normalized RMSE (Dakota/python)

. Calibrated model for different experiments at different temperatures
. Results of sensitivity analysis

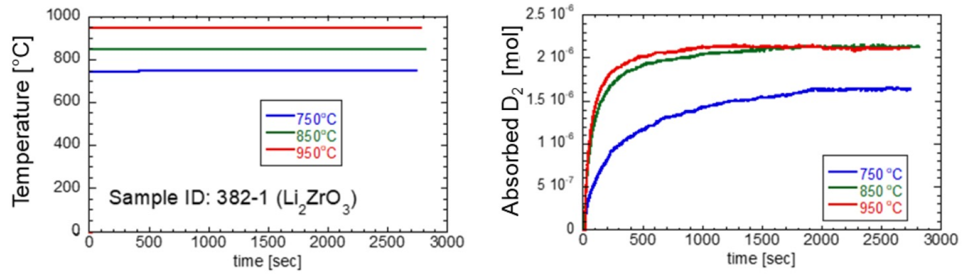


Figure 53: Measured deuterium absorption behavior of 82% dense Li_2ZrO_3 cellular breeder sample SN382-1 at 720 – 730 Pa deuterium pressure (INL).

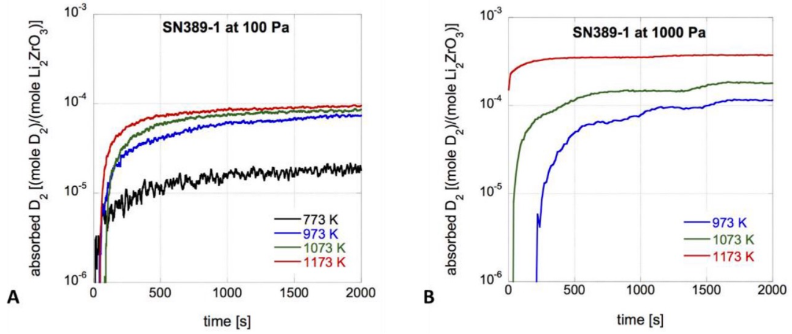


Figure 58A-B: Deuterium absorption behavior of Li_2ZrO_3 cellular breeder (SN389-1; 90% dense) at 100 Pa (A) and (B) 1,000 Pa.

M. Shimada, "Deuterium Absorption and Desorption Behavior in Cellular Solid Breeder Material in support for SBIR Phase II project: 'System Integration and Testing of Robust Cellular Solid Breeder Material with Enhanced Tritium Production and Release," Idaho National Laboratory, Idaho Falls, ID, USA, 2018.

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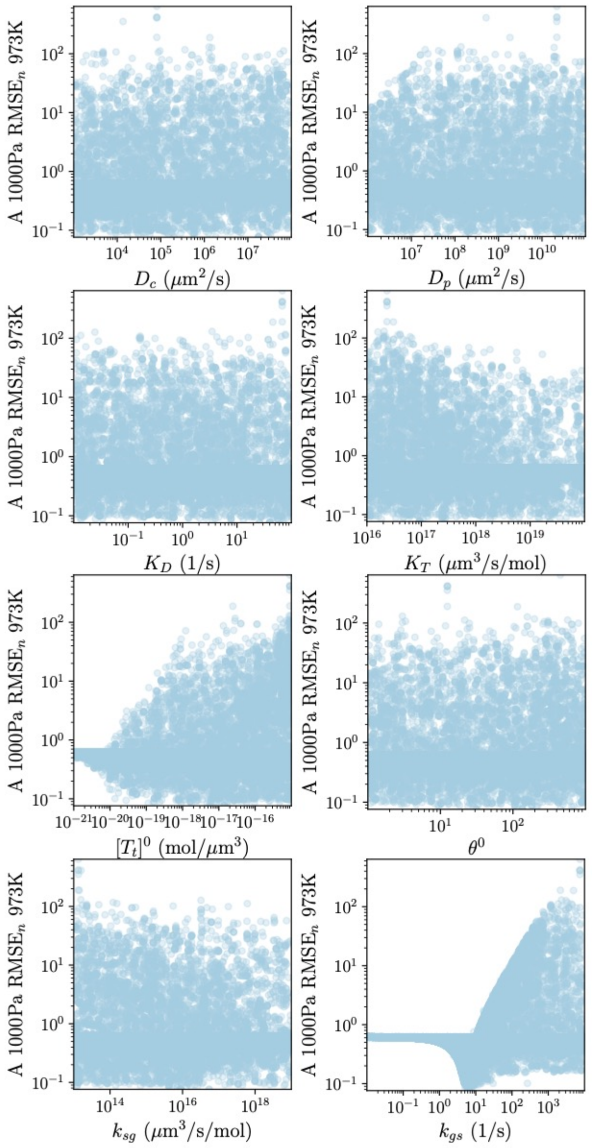
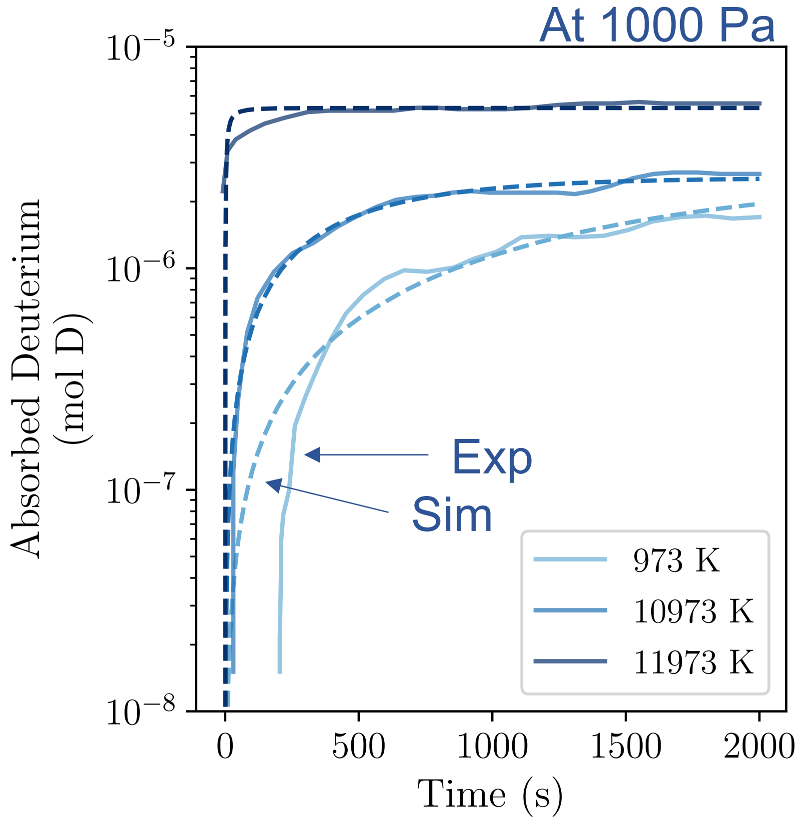
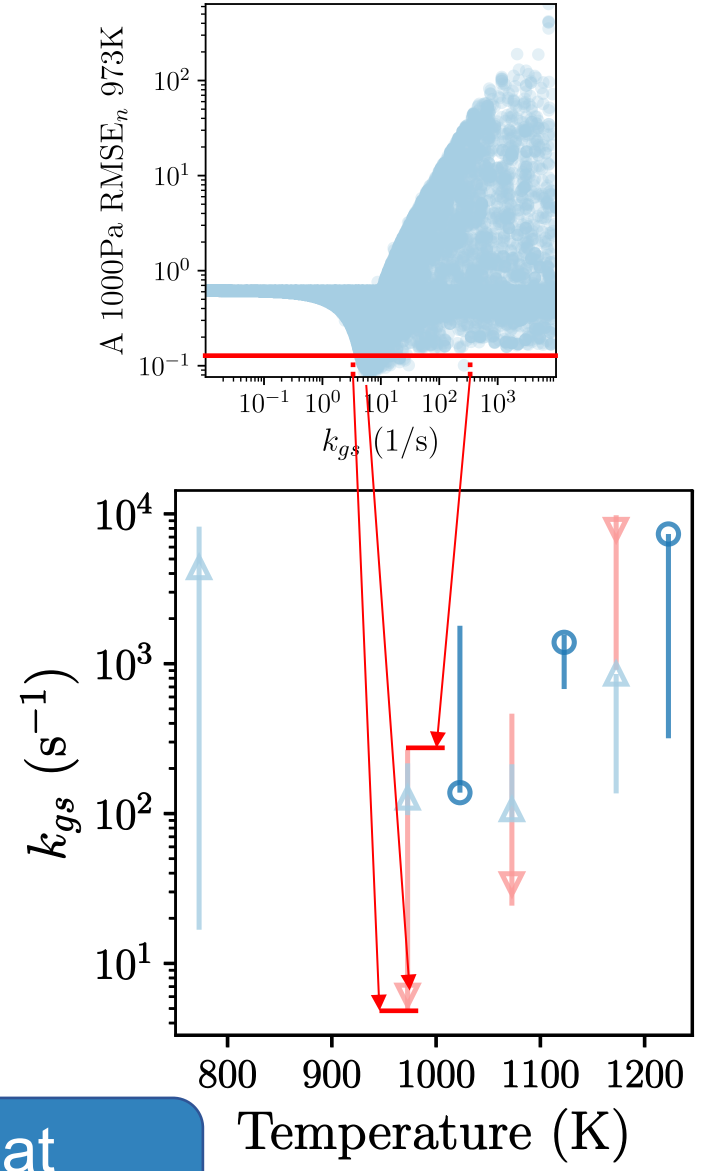
Model Calibration

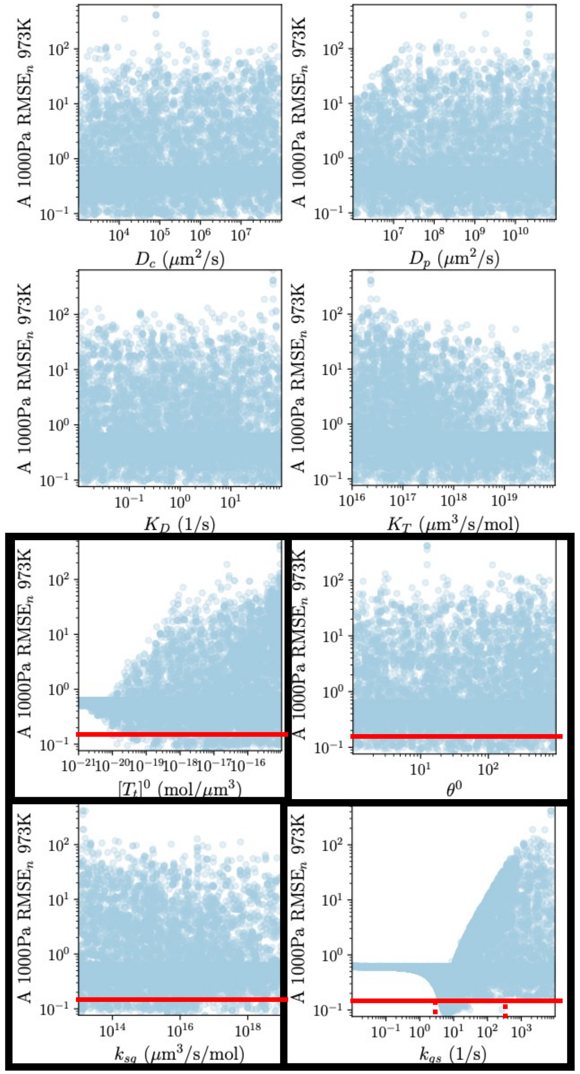


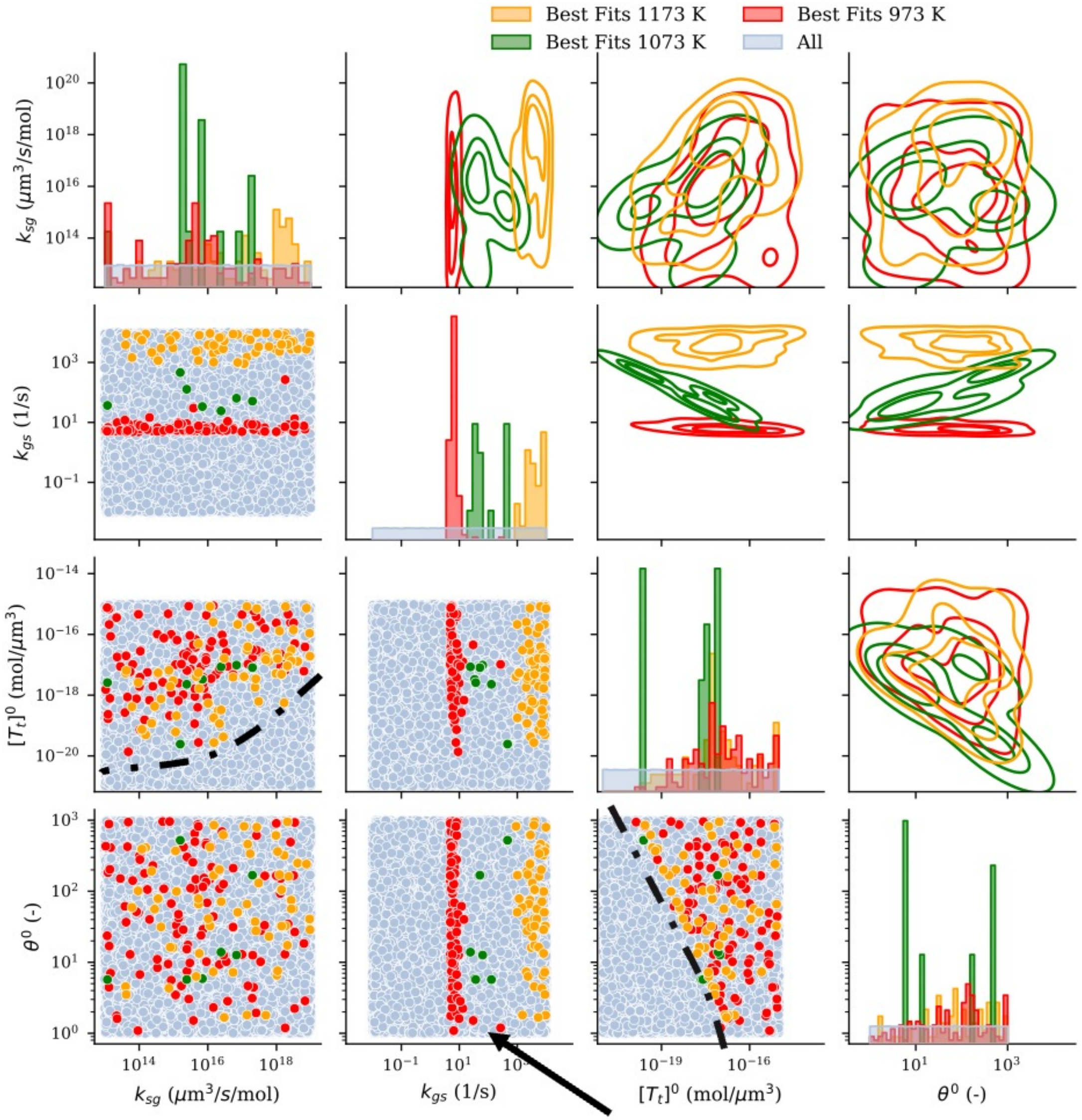




The model was calibrated at different temperatures

Model Sensitivity Study

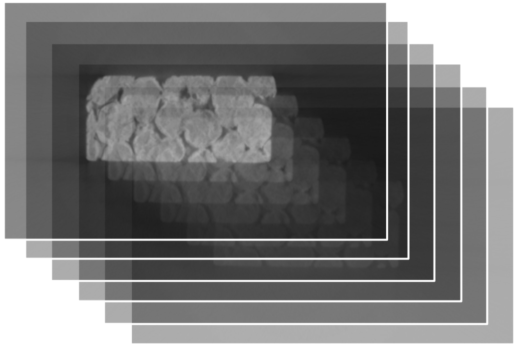




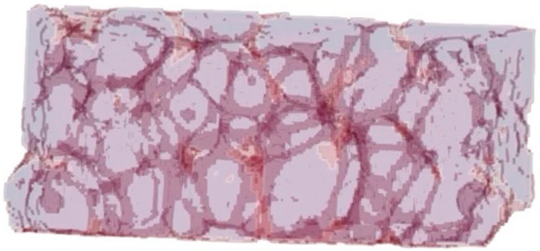
Sensitive parameters and interactions were identified

Enabling 2D and 3D Simulations in Real CCB Pore Structure with TMAP8

2D images of 3D material



Reconstruct 2D/3D microstructure

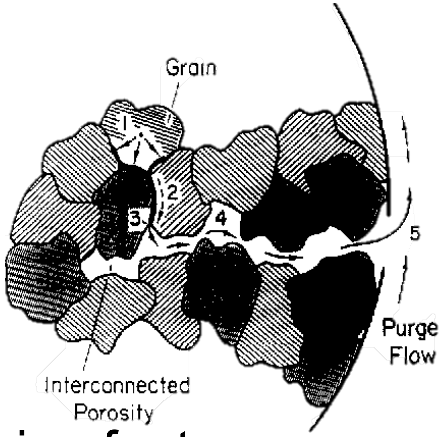


Generated 2D/3D microstructures with lower interconnectivity

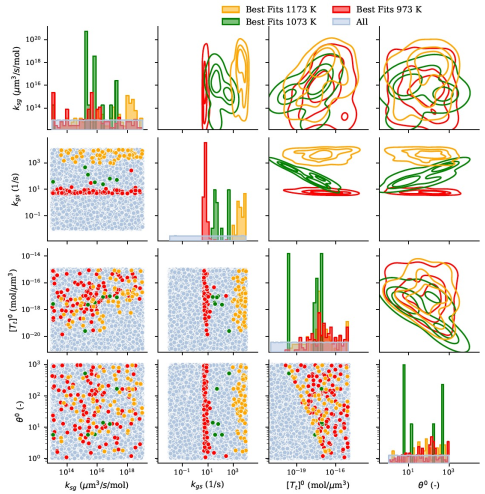
The goal is to show that the 3D pore structure affects tritium transport, and quantify that effect for CCB.

2D images courtesy of Ultramet

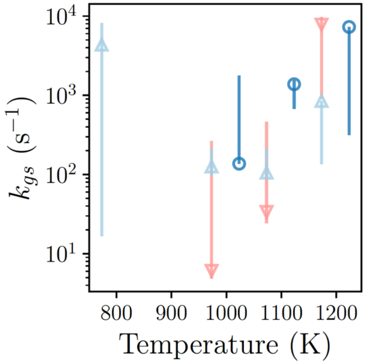
Conclusions and Future Work

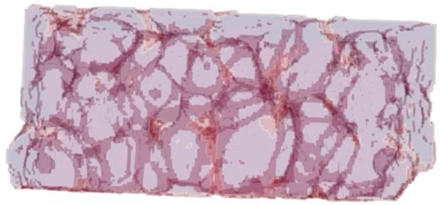


- Conclusions
  - TMAP8 is being developed to model tritium transport using features already implemented in MOOSE
  - A model for tritium transport at the pore scale is being developed
  - The sensitivity of the model is quantified, and the model has been calibrated using experimental data. Leading for temperature-dependent suggestions for model parameters.
  - 3D simulations are enabled



- Future work
  - Finish model calibration (with more experimental data, in particular desorption)
  - Validate model for in-pile experiments
  - Connect the model to the macroscale
    - Derive effective properties to be used at the macroscale
    - Set up multi-scale simulations





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Questions?

Extra: Modeling of Surface Chemical Reactions

<u>Surface Reactions:</u>

Diatomic molecules attaching to the surface

$$H2_g \rightarrow 2\,H_s \;\; rate: K_{d,g\rightarrow s}[H2](1-\theta)^2$$
$$HT_g \rightarrow H_s + T_s \;\; rate: K_{d,g\rightarrow s}[HT](1-\theta)^2$$
$$\mathrm{T}2_\mathrm{g} \rightarrow 2\,T_s \;\; rate: K_{d,g\rightarrow s}[T2](1-\theta)^2$$

Diatomic molecules combining at the surface

$$2\,H_s \rightarrow H2_g \; rate: K_{d,s\rightarrow g}\,[H]^2$$
$$T_s + H_s \rightarrow HT_g \;\; rate: K_{d,s\rightarrow g}\,[H][T]$$
$$2\,T_s \rightarrow T2_g \; rate: K_{d,s\rightarrow g}\,[T]^2$$

Triatomic molecules attaching to the surface

$$H2O_g \rightarrow 2\,H_s + O_s \;\; rate: K_{t,g\rightarrow s}\,[H2O](1-\theta)^3$$
$$HTO_g \rightarrow H_s + T_s + O_s \;\; rate: K_{t,g\rightarrow s}\,[HTO](1-\theta)^3$$
$$\mathrm{T}2O_g \rightarrow 2\,T_s + O_s \;\; rate: K_{t,g\rightarrow s}\,[T2O](1-\theta)^3$$

Triatomic molecules combining at the surface

$$H_s + T_s + O_s \rightarrow HTO_g \;\; rate: K_{t,s\rightarrow g}\,[H][T][O]$$
$$2T_s + O_s \rightarrow T2O_g \;\; rate: K_{t,s\rightarrow g}[T]^2[O]$$
$$2H_s + O_s \rightarrow H2O_g \;\; rate: K_{t,s\rightarrow g}[H]^2[O]$$

$$\theta = \frac{\Sigma[X_i]}{\theta^0[X_\mathrm{t}]^0}$$

Is the number of available sites