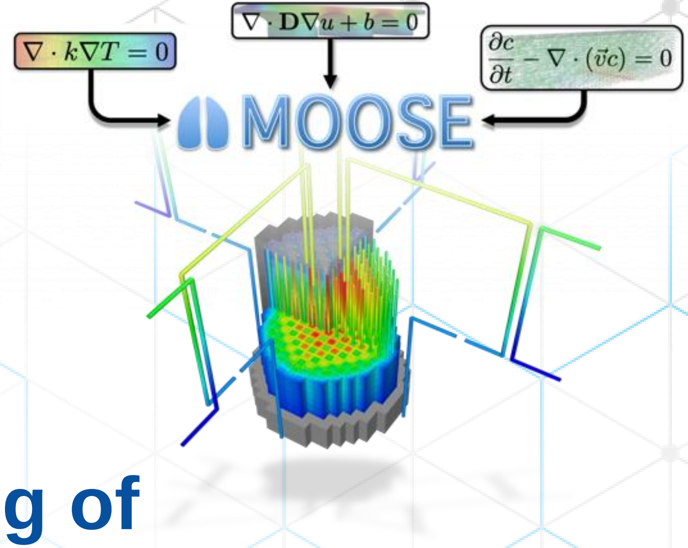
15th International Symposium on Fusion Nuclear Technology (ISFNT-15)
Session: P2 Models & Experiments I



High-fidelity tritium transport modeling of retention and permeation experiment

Masashi Shimada, Casey T. Icenhour, Pierre-Clément A. Simon, and Gyanender Singh

Idaho National Laboratory

INL/CON-23-71901

Tritium Migration Analysis Program (TMAP) is now MOOSE-based:

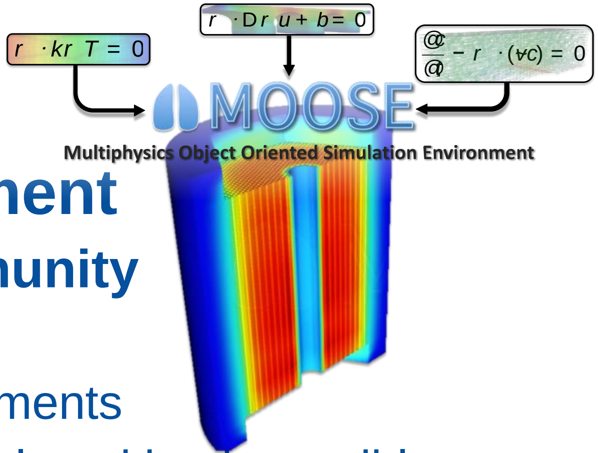
- Open-source
- Free of charge
- Dimension agnostic
- Fully coupled, fully implicit multiphysics solver
- With massively parallel computation (>100,000 CPU cores)

Motivation: TMAP

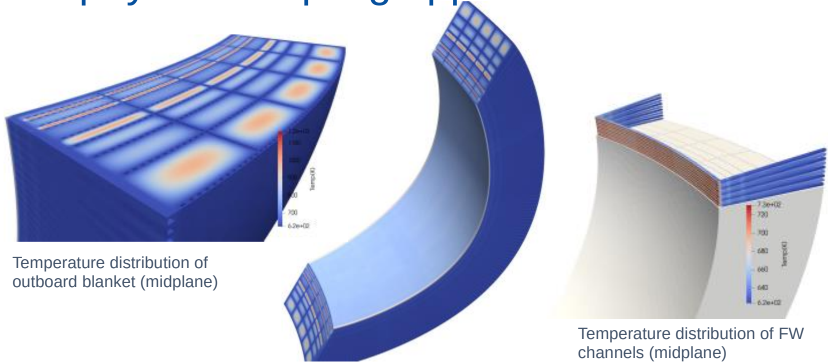
TMAP8 Tritium Migration Analysis Program Version 8”, https://mooseframework.inl.gov/TMAP8/

- **TMAP - Tritium Migration Analysis Program was developed by INL**
  - **Widely used for tritium transport analysis in plasma-facing components & blanket design**
  - **Current capabilities in TMAP4 and TMAP7 are:**
    - TMAP4 (released in 1992) incorporates one-dimensional (1D) thermal- and mass-diffusive transport
      - Trapping calculations (with a single trap) through structures and
      - Zero-dimensional fluid transport between enclosures and across the interface between enclosures & structures.
    - TMAP7 (released in 2006) improved:
      - Trapping model with up to three separate traps,
      - Model for heteronuclear and homonuclear molecule formation, and
      - Surface kinetics calculation with a surface binding energy and an adsorption barrier energy
  - **Challenges in TMAP**
    - Limited to one-dimensional (1D) thermal- and mass-diffusive transport, no 2D/3D modeling capabilities
      - Require significant efforts/funding to add 2D and 3D modeling capabilities in TMAP4/7 (written in Fortran 77)
    - Trapping model capability with up to three separate traps
    - Limited the user support for TMAP4/TMAP7 with man-power (in INL’s Fusion Safety Program)
    - No coupling capabilities with other code, and tritium transport in fusion systems requires multi-physics
    - Limited to single machine, and no parallel computation capability
  - **New version of TMAP8 is MOOSE based** (development started in FY2019 with INL’s PD fund)
    - Several verification & validation problems are available in INL GitHub site.

Motivation: TMAP8 - MOOSE based TMAP



- **MOOSE - Multiphysics Object-Oriented Simulation Environment**
  - **Is developed in INL in 2008 and widely used in nuclear fission community**
    - Open-source framework for development of Multiphysics simulation software
    - Allows rapid development of new simulation tools, and meets NQA-1 requirements
    - Fully coupled and fully implicit multiphysics solver that is automatically parallel, making it possible to run large simulations and tackle complicated models.
  - **“Fission” and “fusion” are very different, but the commonalities are:**
    - Computational material, 1-D thermal-hydraulics, CFD (both finite element and finite volume), Heat transfer, Mechanical/structural, Multiphysics coupling approaches, Native & external applications
  - **Advantage with MOOSE**
    - Massively parallel computations (largest runs >100,000 CPU cores)
    - Coupling capabilities with other MOOSE tools developed for fission:
      - Thermal-hydraulics, CFD, Heat transfer, Mechanical/structural, Multiphysics coupling approaches
    - Dimension agnostics
      - Easy to create 2D/3D modeling with MOOSE
    - Available in GitHub with extensive user support
      - https://mooseframework.inl.gov/
      - https://github.com/idaholab/moose/discussions



Temperature distribution of outboard blanket (midplane)

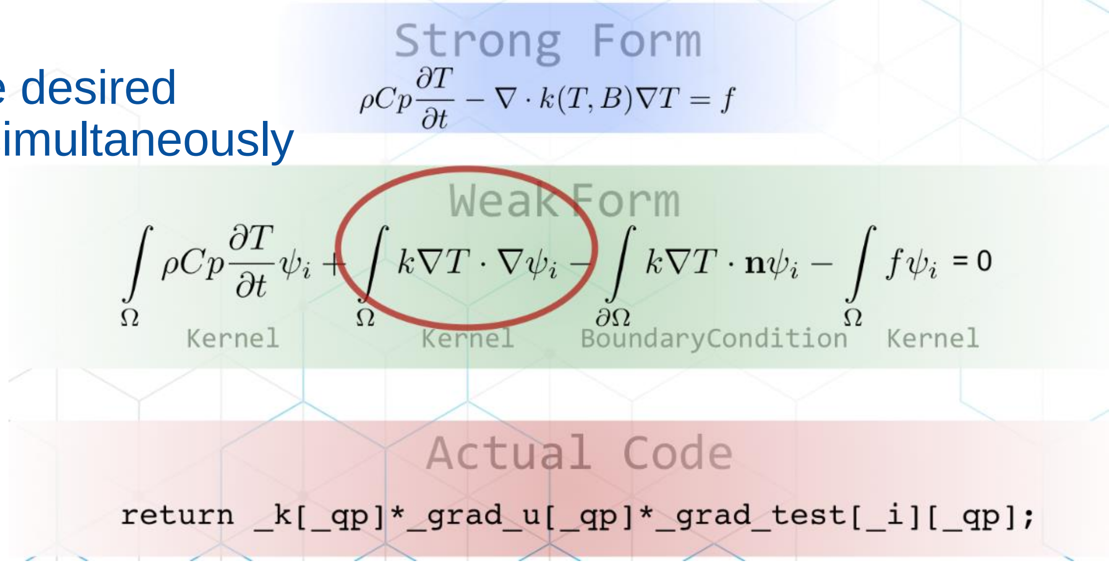
Temperature distribution of FW channels (midplane)

References:
Permann, Cody J., et al. "MOOSE: Enabling massively parallel multiphysics simulation." SoftwareX 11 (2020): 100430.
F. Kong, P.W. Humrickhouse. "Toward a Fully Integrated Multiphysics Simulation Framework for Fusion Blanket Design." IEEE Trans. on Plasma Science (2022).

MOOSE input file

MOOSE Workshop (September 2023), https://mooseframework.inl.gov/workshop/#/

- **TMAP8 (MOOSE-based TMAP) requires:**
  - **Totally different input structure from TMAP4/TMAP7**
  - **Input structures are based on equations (e.g. ODEs, PDEs) to be solved**
  - **MOOSE uses finite element methods (FEM) and requires weak form of PDEs**
    - The weak foam provides flexibility, both mathematically and numerically to solve a problem in MOOSE
  - **General steps to create a weak form from a strong form of PDEs.**
    1) Write down strong form of PDE
    2) Rearrange terms so that zero is on the right of the equal sign
    3) Multiply the whole equation by a “test” function, ψ
    4) Integrate the whole equation over the domain, Ω
    5) Integrate by parts and use the divergence to get the desired derivative order on your functions (i.e. kernel) and simultaneously generate boundary integrals (i.e. BC)



Strong Form

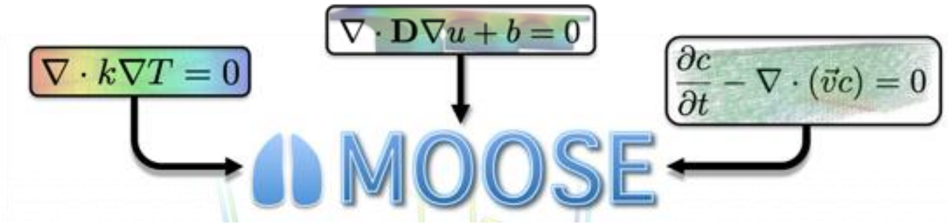
$$\rho C p \frac{\partial T}{\partial t} - \nabla \cdot k(T,B)\nabla T = f$$

Weak Form

$$\int_\Omega \rho C p \frac{\partial T}{\partial t}\psi_i + \int_\Omega k\nabla T \cdot \nabla \psi_i - \int_{\partial\Omega} k\nabla T \cdot \mathbf{n}\psi_i - \int_\Omega f\psi_i = 0$$

Actual Code

```
return _k[_qp]*_grad_u[_qp]*_grad_test[_i][_qp];
```



3D example to model in TMAP8

IOP Publishing | Bureau International des Poids et Mesures — Nuclear Fusion

Nucl. Fusion 61 (2021) 036038 (14pp) — https://doi.org/10.1088/1741-4326/abd95f

Influence of interface conditions on hydrogen transport studies

Rémi Delaporte-Mathurin[1,2,*], Etienne A. Hodille[1], Jonathan Mougenot[2], Yann Charles[2], Gregory De Temmerman[3], Floriane Leblond[1] and Christian Grisolia[1]

- **Tritium transport in monoblock**
  - **<u>2D</u> tritium & thermal transport by FESTIM code**
    - Remi Delaporte-Mathurin *et al. 2021 Nuclear Fusion*
    - 1D (8.5mm W/Cu/CuCrZr) and 2D (28mm x 28mm monoblock)
    - No ion implantation with volumetric source term in first few nm
    - Boundary condition (Dirichlet BC):
      - $300 < T_{surface}$ [K]< 1200,
      - $10^{20} < c_{surface}$ [m^{-3}] $< 6 \times 10^{22}$ ➔ $10^{-9} < c_{surface}$ [T/W] $< 10^{-6}$

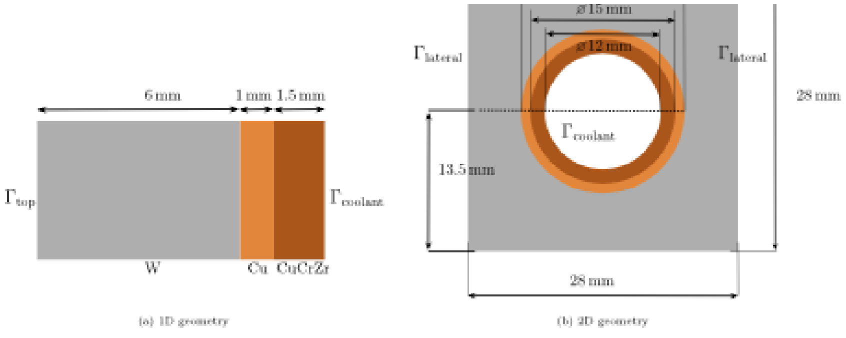
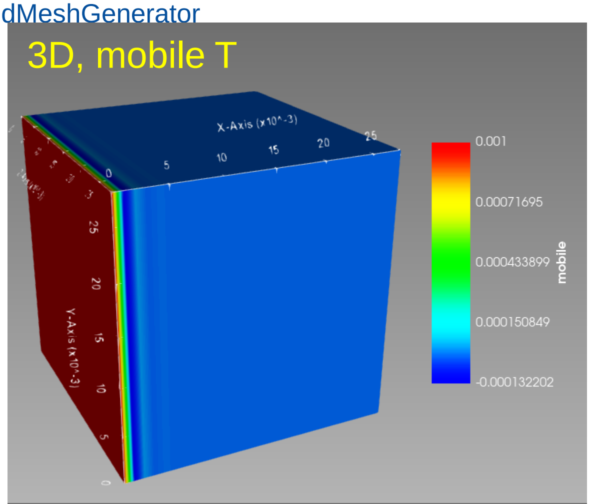


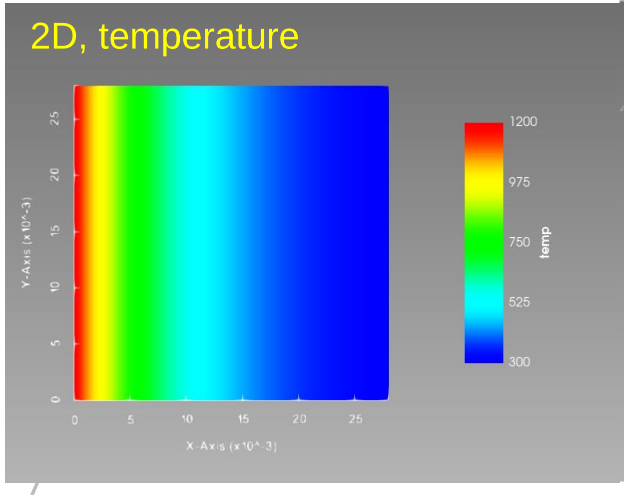
Figure 5. Monoblock geometry showing W armour d1, Cu interlayer d2, CuCrZr alloy cooling pipe d3.

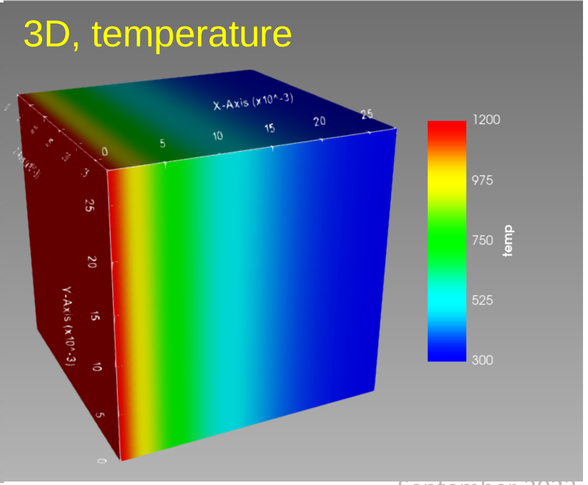
- **The scope of this work:**
  - **Perform tritium and heat transport modeling in <u>3D</u> geometry with TMAP8**
    - Tritium and heat transport in a single material with W (instead of W/Cu/CuCrZr)
    - Simplified boundary condition used for plasma implantation
  - **Simulate plasma on/off scenario (600 sec plasma on, 1000 sec plasma off) up to 100 shots**
    - Demonstrate ITER-like on/off scenario
- **NOTE:**
  - **This is still <u>qualitative</u> analysis, not quantitative yet. Further V&V of TMAP8 is necessary.**
  - **The purpose is to show the potential of TMAP8 for high-fidelity tritium transport modeling**
  - **This work is done with TMAP8 with a single machine.**

Simplified monoblock geometry in TMAP8

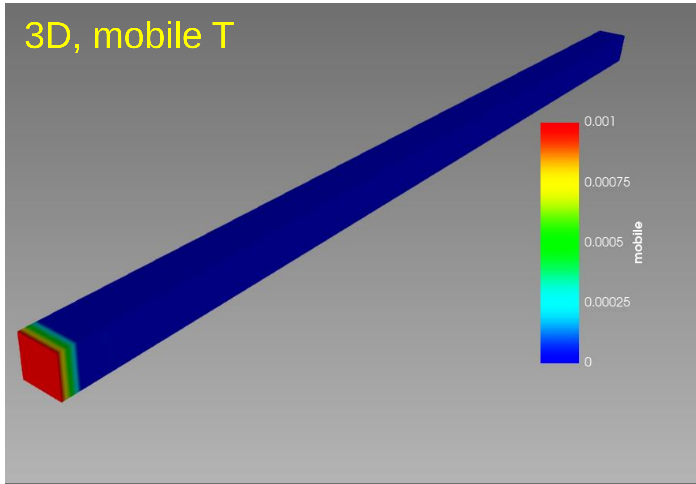
- **3D geometry (28x28x28mm^3)**
  - **56 nodes per sides**
  - **Requires parallel computing or HPC**
  - **TMAP input file**
    - [3d_mesh]
      - type = GeneratedMeshGenerator
      - dim = 3
      - nx = 56
      - ny = 56
      - nz = 56
      - xmin = 0
      - xmax = 28.0e-3
      - ymin = 0
      - ymax = 28.0e-3
      - zmin = 0
      - zmax = 28.0e-3
    - []

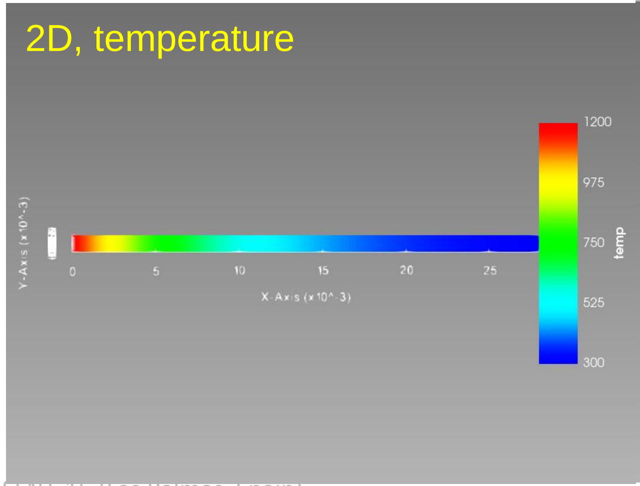

3D, mobile T

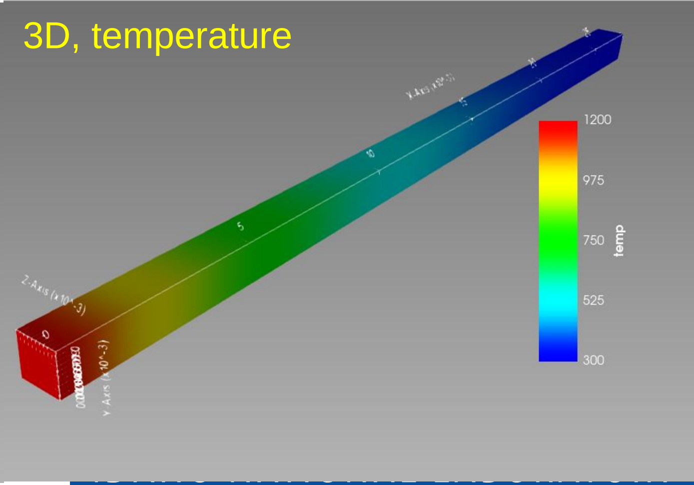

2D, temperature


3D, temperature

- **Simplified 3D geometry (28x1x1mm^3)**
  - **This can be performed by a single machine**
  - **TMAP input file**
    - [3d_mesh]
      - type = GeneratedMeshGenerator
      - dim = 3
      - nx = 56
      - ny = 2
      - nz = 2
      - xmin = 0
      - xmax = 28.0e-3
      - ymin = 0
      - ymax = 1.0e-3
      - zmin = 0
      - zmax = 1.0e-3
    - []


3D, mobile T


2D, temperature


3D, temperature

Equations to solve for tritium transport in metal

- **Conservation of mass for solute gas atom (s = H, D, T)**

$$\frac{\partial C_s}{\partial t} + \nabla \cdot J_s = S_s - \frac{\partial C_s^t}{\partial t}$$

Strong form

Step (2)

$$\frac{\partial C_s}{\partial t} + \nabla \cdot J_s + \frac{\partial C_s^t}{\partial t} - S_s = 0$$

$$\frac{\partial C_s}{\partial t} + \nabla \cdot (-D_s \nabla C_s) + \frac{\alpha_{t_s} C_t^e}{N} C_s - \alpha_{r_s} C_s^t = 0$$

Step (3)

$$\psi \frac{\partial C_s}{\partial t} - \psi(\nabla \cdot D_s \nabla C_s) + \psi \frac{\alpha_{t_s} C_t^e}{N} C_s - \psi \alpha_{r_s} C_s^t = 0$$

Step (4)

$$\int_\Omega \psi \frac{\partial C_s}{\partial t} - \int_\Omega \psi(\nabla \cdot D_s \nabla C_s) + \int_\Omega \psi \frac{\alpha_{t_s} C_t^e}{N} C_s - \int_\Omega \psi \alpha_{r_s} C_s^t = 0$$

Insert the following assumptions

$$S_s = 0$$

$$J_s = -D_s \left[\nabla C_s + \frac{Q_s^* C_s}{RT^2} \nabla T \right] = -D_s \nabla C_s$$

$$\frac{\partial C_s^t}{\partial t} = \frac{\alpha_{t_s} C_t^e}{N} C_s - \alpha_{r_s} C_s^t$$

where

$$C_t^e = C_t^0 - C_s^t$$

$$\alpha_{t_s} = \frac{D_s}{\lambda^2}$$

$$\alpha_{r_s} = \nu_0 exp\left[-\frac{E_t}{RT} \right]$$

Equations to solve for tritium transport in metal

- **Conservation of mass for solute gas atom (s = H, D, T)**

$$\int_{\Omega} \psi \frac{\partial C_s}{\partial t} - \int_{\Omega} \psi(\nabla \cdot D_s \nabla C_s) + \int_{\Omega} \psi \frac{\alpha_{t_s} C_t^e}{N} C_s - \int_{\Omega} \psi \alpha_{r_s} C_s^t = 0$$

Step (5)

$$\int_{\Omega} \psi \frac{\partial C_s}{\partial t} - \int_{\partial\Omega} \psi\, D_s \nabla C_s \cdot \hat{n} + \int_{\Omega} \nabla\psi \cdot D_s \nabla C_s + \int_{\Omega} \psi \frac{\alpha_{t_s} C_t^e}{N} C_s - \int_{\Omega} \psi \alpha_{r_s} C_s^t = 0$$

Weak form

$$\underbrace{\left(\psi, \frac{\partial C_s}{\partial t}\right)}_{\mathit{Kernel}} - \underbrace{(\psi, D_s\, \nabla C_s \cdot \hat{n})}_{\mathit{Boundary\ Condition\ (BC)}} + \underbrace{(\nabla\psi, D_s \nabla C_s)}_{\mathit{Kernel}} + \underbrace{\left(\psi, \frac{\alpha_{t_s} C_t^e}{N} C_s\right)}_{\mathit{Kernel}} - \underbrace{(\psi, \alpha_{r_s} C_s^t)}_{\mathit{Kernel}} = 0$$

Inner product notation

Examples of
MOOSE Input File Syntax

ADTimeDerivative

FunctionNeumannBC

ADMatDiffusion

TrappingNodalKernel

ReleasingNodalKernel

Equations to solve for heat transport by conduction

Complete TMAP8 Input File Syntax, https://mooseframework.inl.gov/TMAP8/syntax/

- **Conservation of energy**

$$\rho C_p \frac{\partial T}{\partial t} = -\nabla \cdot q + \dot{q_v}$$

Strong form

Step (2)

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot q - \dot{q_v} = 0$$

Insert the following assumptions

$$\dot{q_v} = 0$$

$$q = -k_T \nabla T$$

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k_T \nabla T) = 0$$

Step (3)

$$\psi\, \rho C_p \frac{\partial T}{\partial t} - \psi(\nabla \cdot k_T \nabla T) = 0$$

Step (4)

$$\int_{\Omega} \psi \rho C_p \frac{\partial T}{\partial t} - \int_{\Omega} \psi(\nabla \cdot k_T \nabla T) = 0$$

Equations to solve for heat transport by conduction

Complete TMAP8 Input File Syntax, https://mooseframework.inl.gov/TMAP8/syntax/

- **Conservation of energy**

$$\int_{\Omega} \psi \rho C_p \frac{\partial T}{\partial t} - \int_{\Omega} \psi (\nabla \cdot k_T \nabla T) = 0$$

← Step (5)

$$\int_{\Omega} \psi \rho C_p \frac{\partial T}{\partial t} - \int_{\partial\Omega} \psi k_T \nabla T \cdot \hat{n} + \int_{\Omega} \nabla\psi \cdot k_T \nabla T = 0$$

Weak form

$$\underbrace{\left(\psi, \rho C_p \frac{\partial T}{\partial t}\right)}_{Kernel} - \underbrace{(\psi, k_T \,\nabla T \cdot \hat{n})}_{\substack{Boundary\ Condition \\ (BC)}} + \underbrace{(\nabla\psi, k_T \nabla T)}_{Kernel} = 0$$

Inner product notation

SpecificHeatConductionTimeDerivative

FunctionDirichletBC

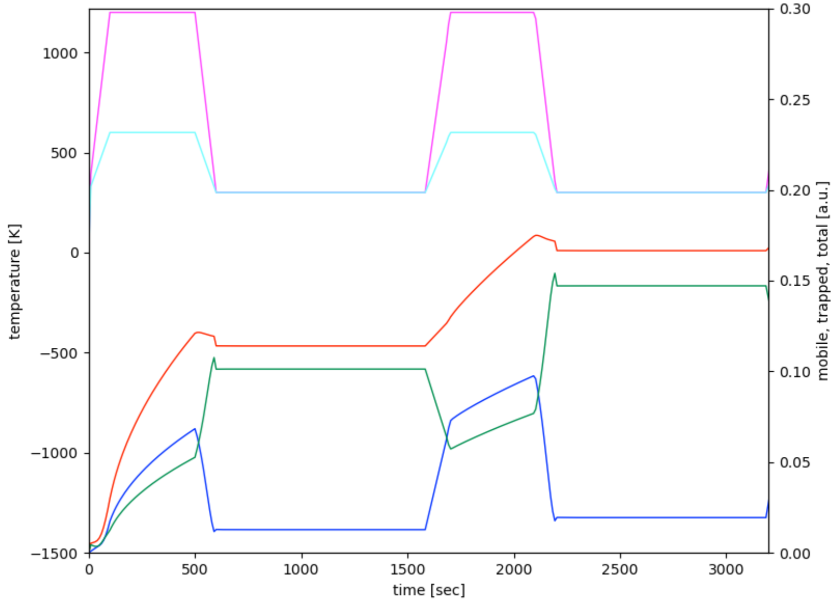
HeatConduction

Examples of
MOOSE Input File Syntax

Preliminary results in TMAP8 (qualitative results)

- **Tritium inventory modeling in 2, 10, and 100 plasma on/off scenario**
  - **Total inventory of tritium (in red), mobile tritium (in blue) and trapped tritium (in green)**

First 2 shots, temperature (top)
total tritium, mobile and trapped (bottom)



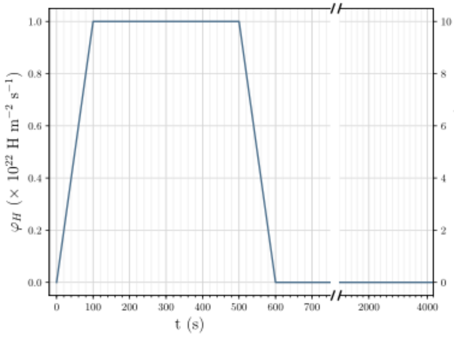
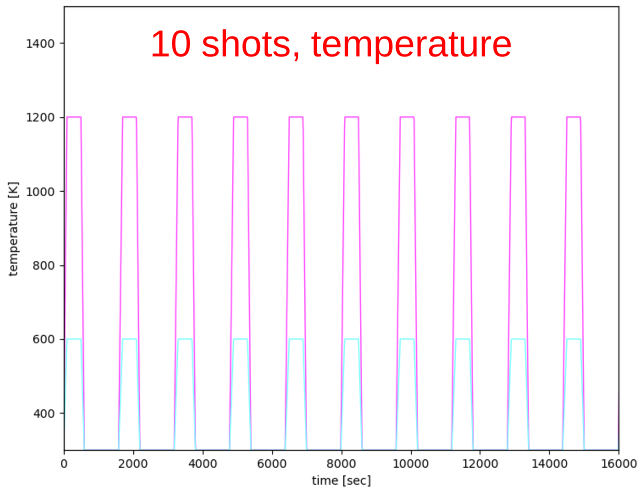
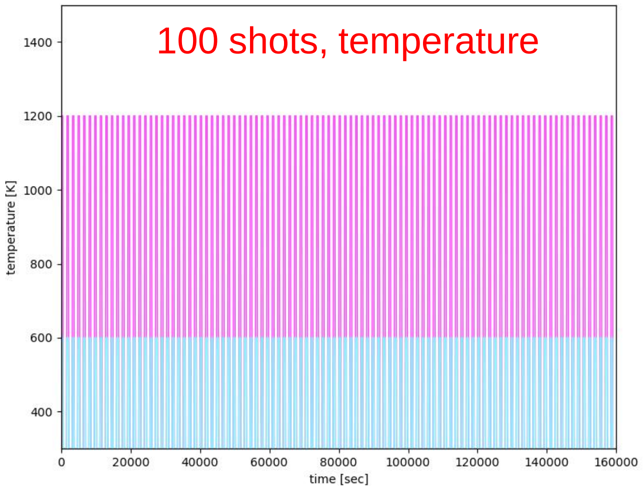


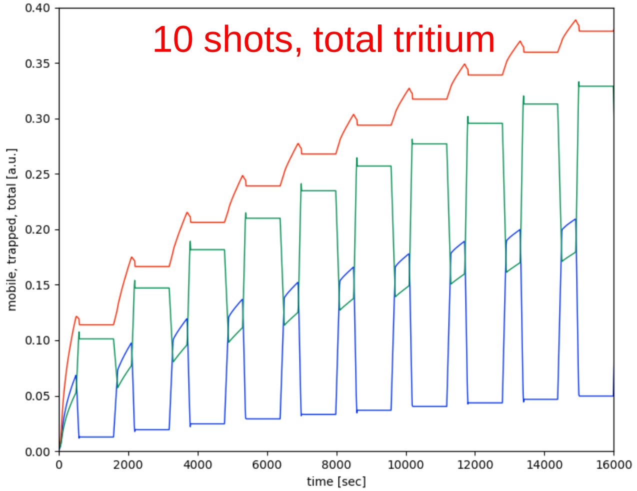
Fig. 5. Evolution of φ_T and φ_H during one plasma cycle.

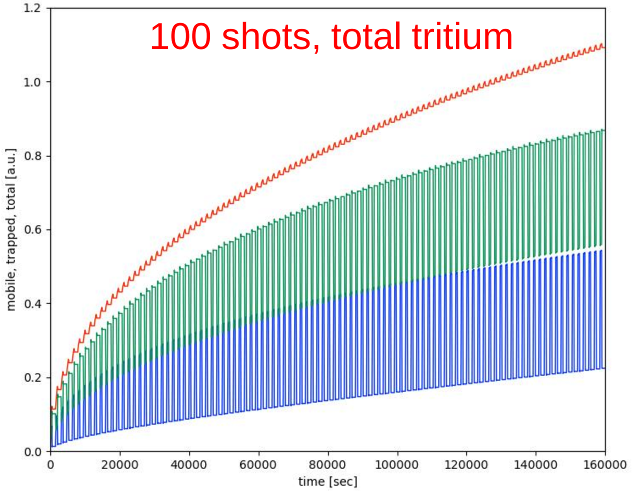
Temperature profile
ITER 1 shot

References:
R. Delaporte-Mathurin et al,
Nucl. Mater. Energy **21** (2019) 100709


10 shots, temperature

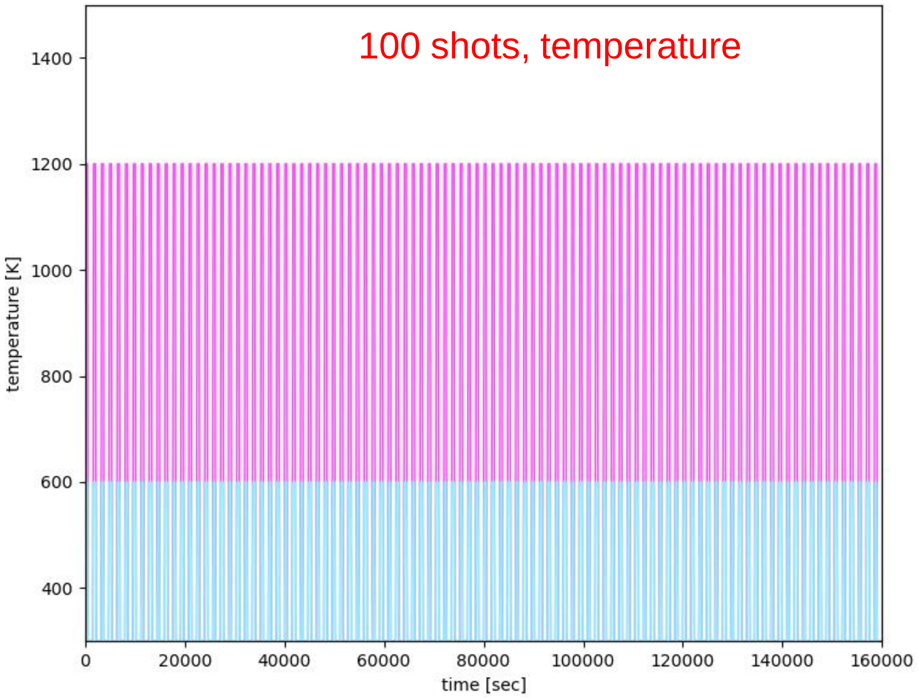

100 shots, temperature

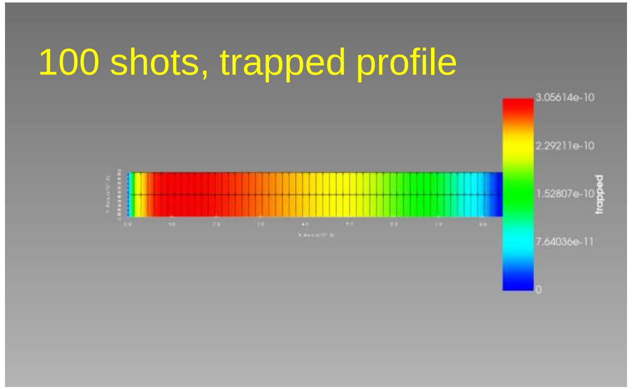

10 shots, total tritium

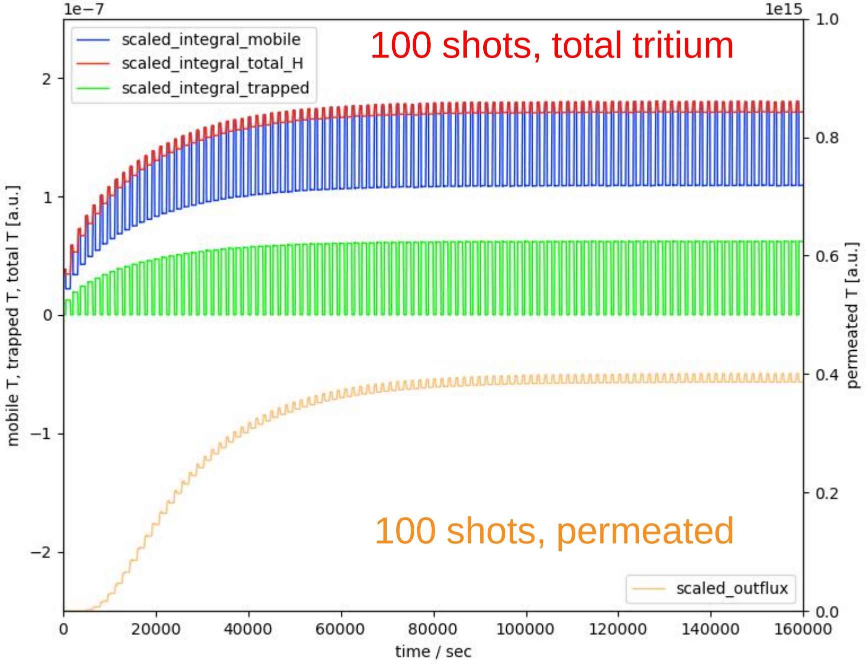

100 shots, total tritium

Preliminary results in TMAP8 (qualitative results)

- **Tritium inventory modeling in 100 plasma on/off scenario**
  - **Total inventory of tritium (in red), mobile tritium (in blue) and trapped tritium (in green)**
  - **Trapped T profile at 10 and 100 shots**
- **Tritium permeation modeling in 100 plasma on/off scenario**
  - **Tritium permeation flux to the coolant shows typical transient and steady state permeation profile**

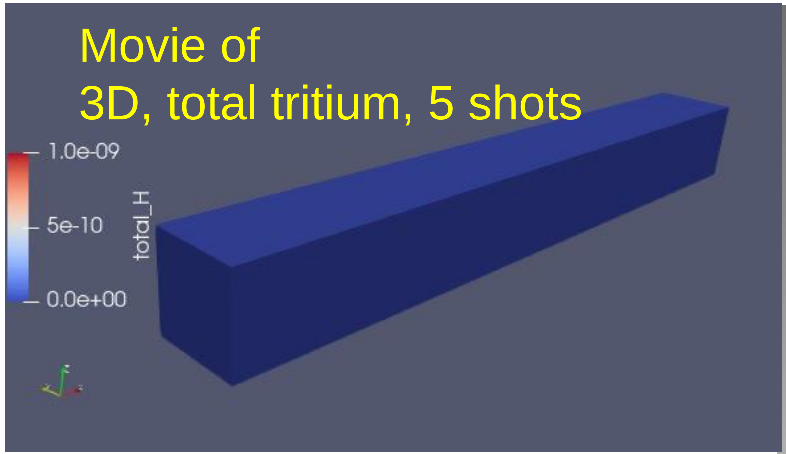


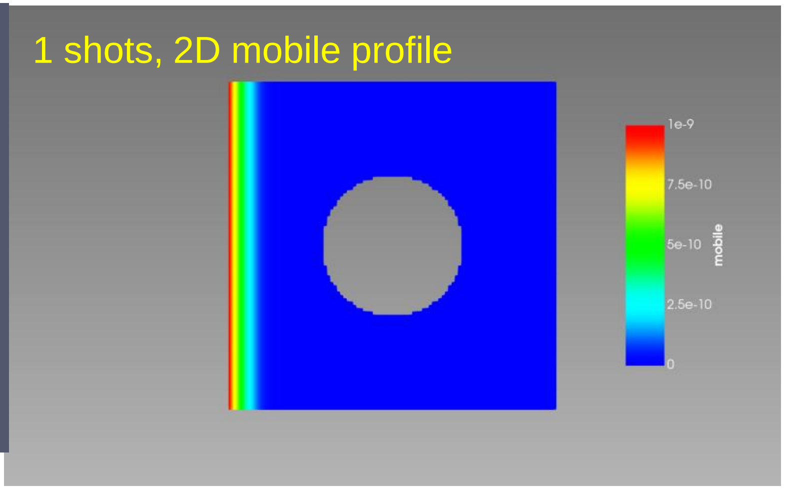


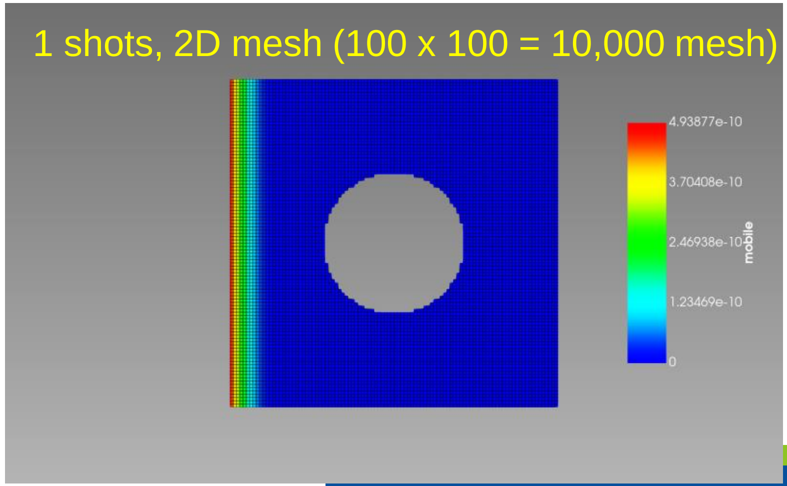


Summary and future work

- **MOOSE-based TMAP8 shows:**
  - **Promising modeling capabilities for high-fidelity tritium transport in 3D geometry**
    - Leverage MOOSE framework and MOOSE tools developed for nuclear fission application
    - Extremely easy to allow 2D and 3D modeling with simple change in TMAP input file
    - Extensive users support for TMAP8
  - **Status of TMAP8**
    - Verification & Validation (V&V) is underway at https://mooseframework.inl.gov/TMAP8/
    - 7 verification cases were completed and 1 validation case was completed from TMAP4 V&V examples
  - **Future work**
    - Further development and V&Vs are necessary to perform quantitative analysis of tritium transport
    - Couple TMAP8 with other MOOSE tools and apps and perform modeling with parallel computation

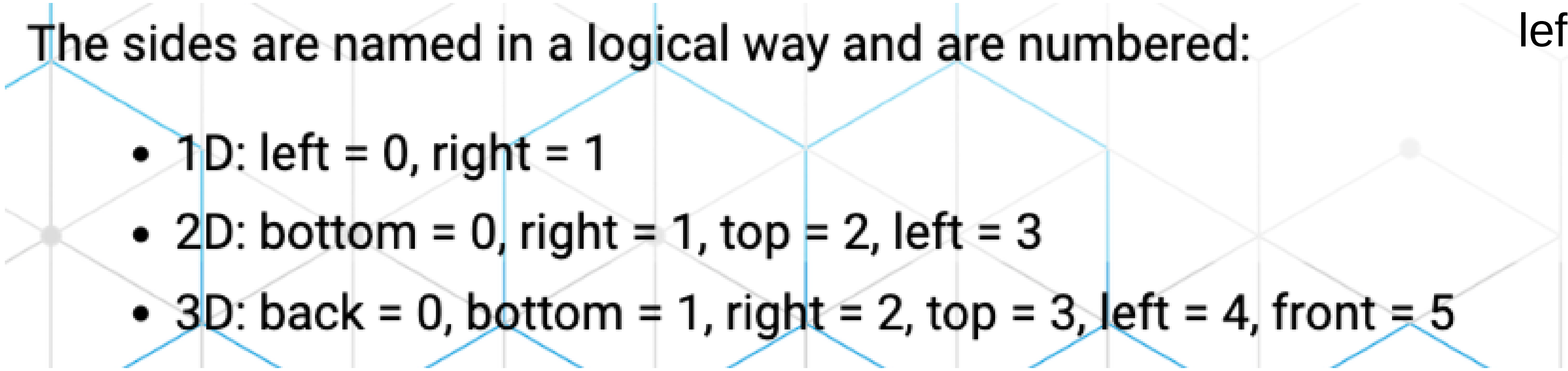

Movie of
3D, total tritium, 5 shots


1 shots, 2D mobile profile


1 shots, 2D mesh (100 x 100 = 10,000 mesh)

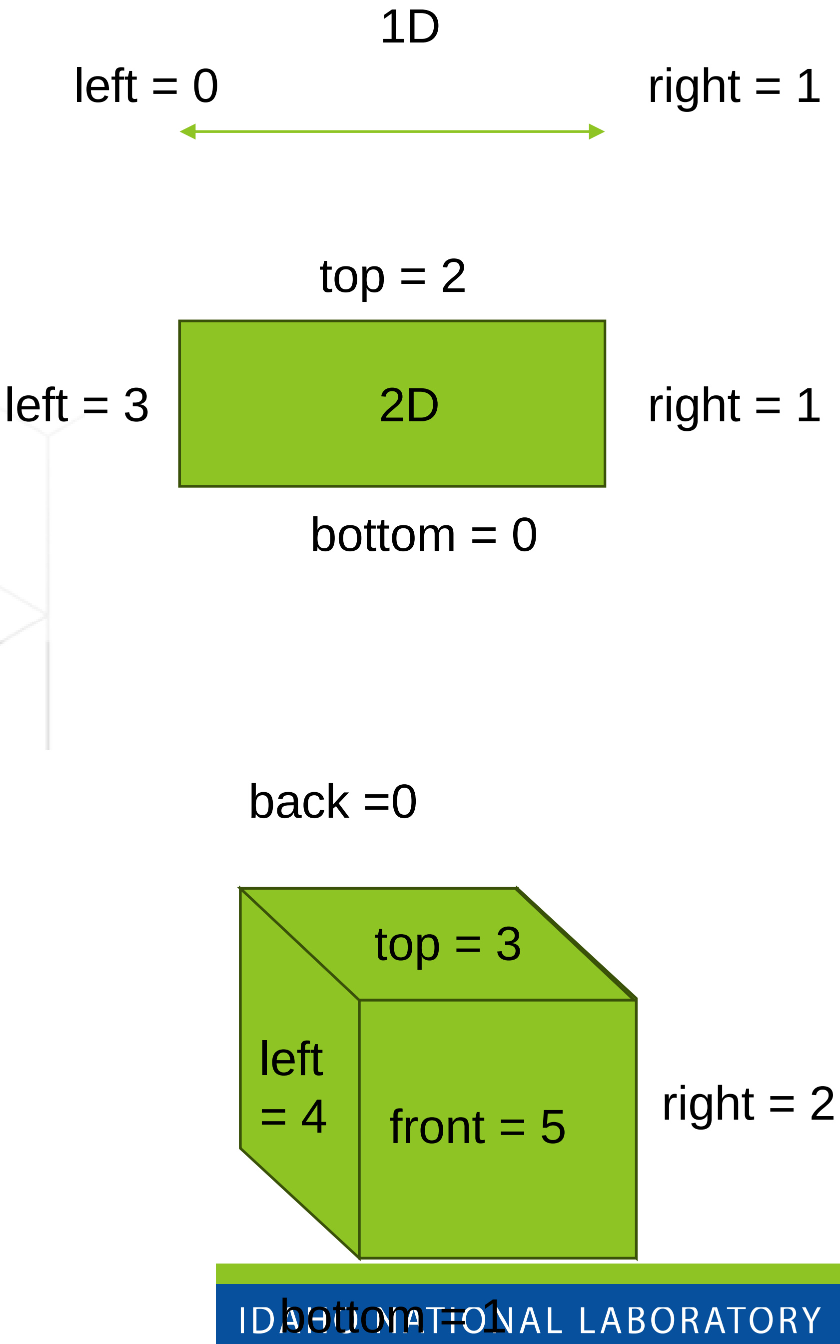
Extra slides

1D, 2D, and 3D boundaries



The sides are named in a logical way and are numbered:

- 1D: left = 0, right = 1
- 2D: bottom = 0, right = 1, top = 2, left = 3
- 3D: back = 0, bottom = 1, right = 2, top = 3, left = 4, front = 5



1D

left = 0

right = 1

top = 2

left = 3

2D

right = 1

bottom = 0

back =0

top = 3

left = 4

front = 5

right = 2

bottom = 1

TMAP8: FY2018-2023 accomplishments: verification

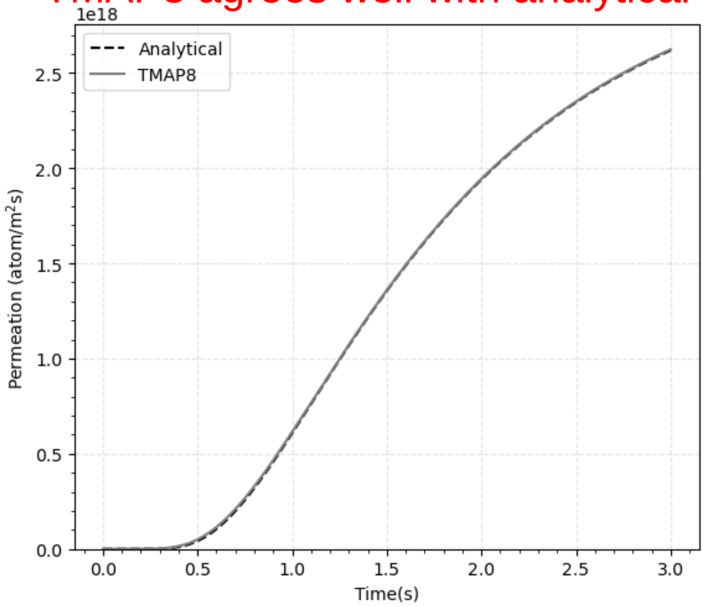
- **Verification example: Ver-1d, “Permeation Problem with Trapping”**
  - It models permeation through a membrane with a constant source in which traps are operative.
  - The breakthrough time may have one of two limiting values depending on whether the trapping is in the effective diffusivity or strong-trapping regime.
  - A trapping parameter is defined by.

$$\zeta = \frac{\lambda^2 \nu}{\rho D_0} exp\left(\frac{E_d - \varepsilon}{kT}\right) + \frac{c}{\rho}$$

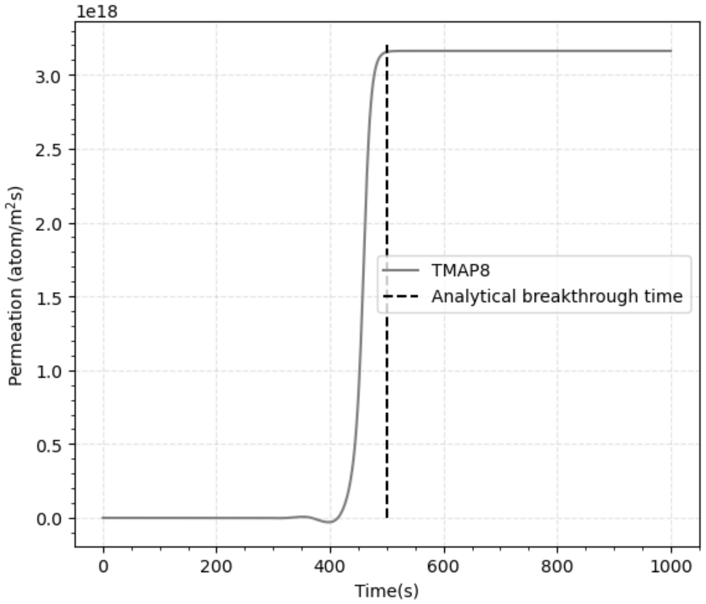
λ = lattice parameter
ν = Debye frequency ($\approx 10^{13}\ s^{-1}$)
ρ = trapping site fraction
D_o = diffusivity pre-exponential
E_d = diffusion activation energy
ϵ = trap energy
k = Boltzmann's constant
T = temperature
c = dissolved gas atom fraction

TMAP8 agrees well with analytical

$$\zeta = 91.47\, c/\rho$$



1D



$$\zeta = 1.0045\, c/\rho$$

1D

Diffusion-limited in effective diffusivity regime, $\zeta \gg c/\rho$,

Trap-limited in deep-trapping regime, $\zeta \approx c/\rho$,

Reference:

GR Longhurst, SL Harms, ES Marwil, and BG Miller. Verification and validation of tmap4. Technical Report, EG and G Idaho, Inc., Idaho Falls, ID (United States), 1992.
TMAP8 V&V ver-1d, https://mooseframework.inl.gov/TMAP8/verification/ver-1d.html#longhurst1992verification

TMAP8: FY2018-2023 accomplishments: verification

- **Verification example: Ver-1d, “Permeation Problem with Trapping”**
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  - The breakthrough time may have one of two limiting values depending on whether the trapping is in the effective diffusivity or strong-trapping regime.
  - A trapping parameter is defined by.

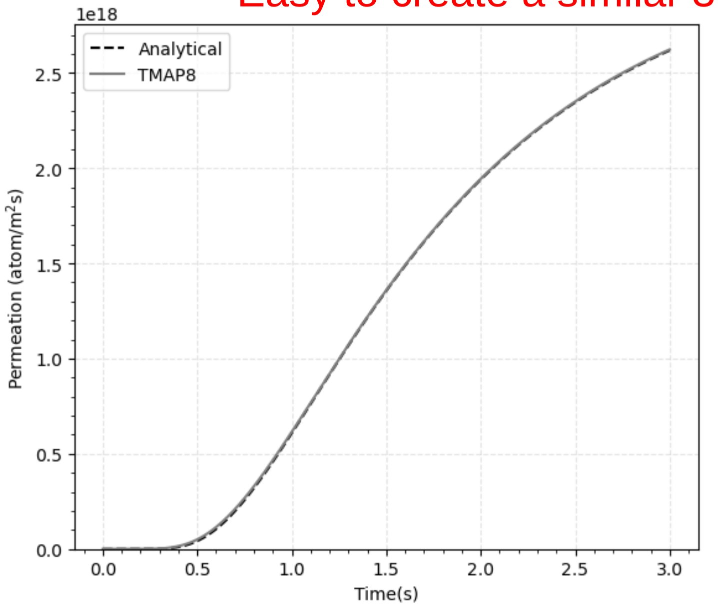
$$\zeta = \frac{\lambda^2 \nu}{\rho D_0} exp\left(\frac{E_d - \varepsilon}{kT}\right) + \frac{c}{\rho}$$

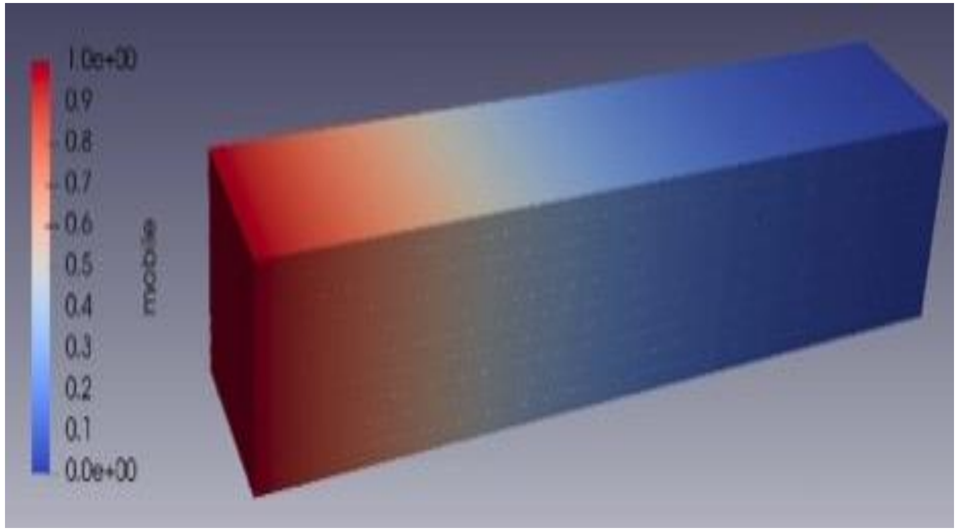
λ = lattice parameter
ν = Debye frequency ($\approx 10^{13}\ s^{-1}$)
ρ = trapping site fraction
D_o = diffusivity pre-exponential
E_d = diffusion activation energy
ϵ = trap energy
k = Boltzmann's constant
T = temperature
c = dissolved gas atom fraction

Easy to create a similar 3D model from 1D model in MOOSE

$\zeta = 91.47\ c/\rho$

1D





$\zeta = 91.47\ c/\rho$

3D

Diffusion-limited in effective diffusivity regime, $\zeta \gg c/\rho$,

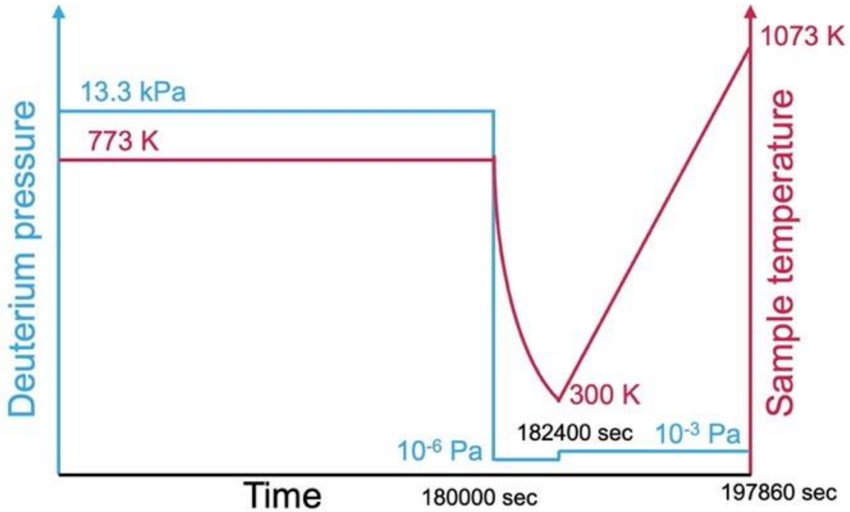
Diffusion-limited in effective diffusivity regime, $\zeta \gg c/\rho$,

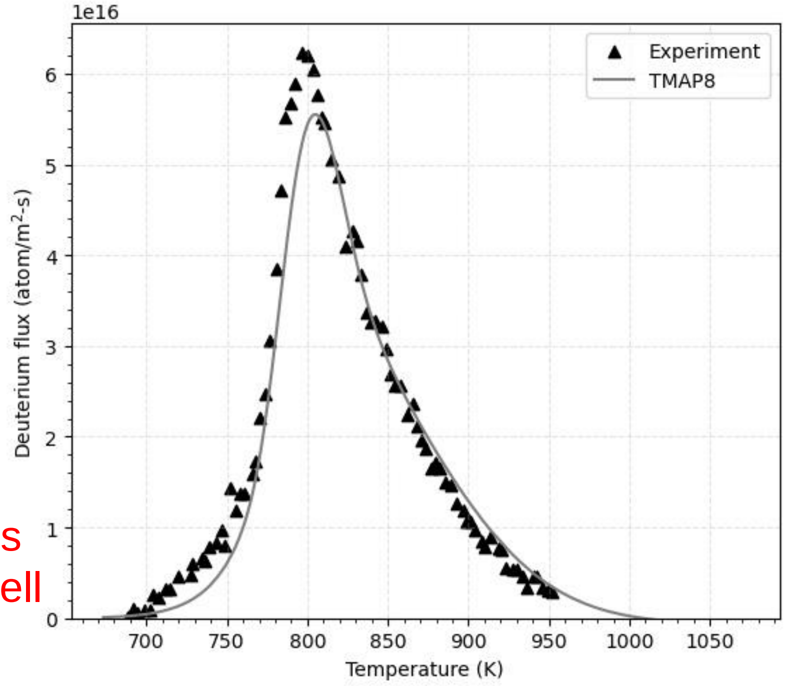
Reference:

GR Longhurst, SL Harms, ES Marwil, and BG Miller. Verification and validation of tmap4. Technical Report, EG and G Idaho, Inc., Idaho Falls, ID (United States), 1992.
TMAP8 V&V ver-1d, https://mooseframework.inl.gov/TMAP8/verification/ver-1d.html#

TMAP8: FY2018-2023 accomplishments: validation

- **Validation example: Val-2b “Diffusion Experiment in Beryllium”**
  - It models thermal absorption and desorption experiments, as well as implantation experiments, on wafers of polished beryllium.
  - D_2 absorption experiment:
    - 0.4 mm thick beryllium sample (surface area: 104 mm^2)
    - Exposed to 13.3 kPa of deuterium at 773 K for 50 hours, and
    - Quickly cooled at 10^{-6} Pa with a time constant of 45 minutes
  - Thermal desorption experiment:
    - From ambient (300 K) to 1073 K at the rate of 3 K/min.





TMAP8 reproduces this diffusion experiment well

Reference:

R.G. Macaulay-Newcombe, et al., “Thermal adsorption and desorption of deuterium in beryllium and beryllium oxide”, J. Nucl. Mater. 191-194 (1992) 263.

TMAP8 V&V val-2b, https://mooseframework.inl.gov/TMAP8/verification/val-2b.html