Multiphysics tritium transport modelling in WCLL breeding blankets: Influence of neutron damage and MHD effects

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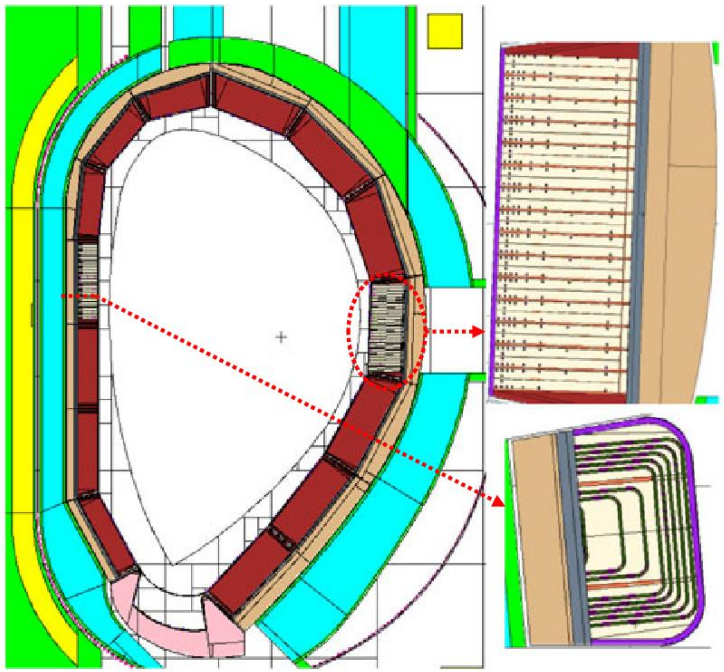
Simulating a WCLL

Water Cooled Lithium Lead



Safety

Strict limitations on tritium inventories in DEMO

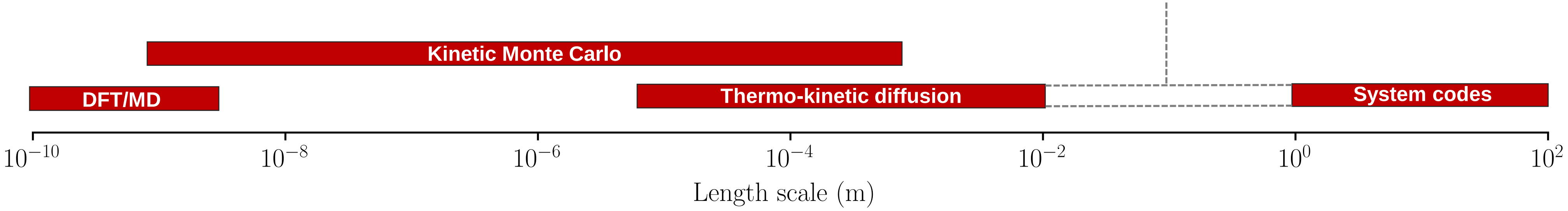
Tritium release into local environment

Performance

To ensure maximum tritium recovery

Length scale of modelling literature

Gap in research

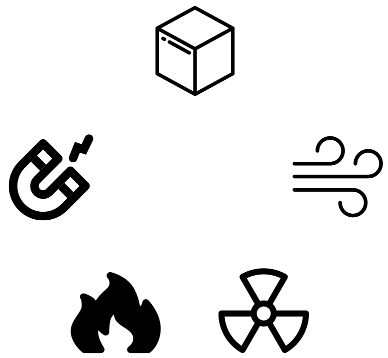


Project Objectives

- To investigate **influencing factors** on hydrogen transport in WCLL breeding blanket for DEMO

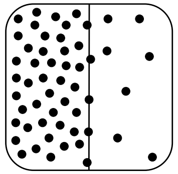
- Suggest **design alterations** to improve breeding blanket performance

Model multi-dimensional, multi-physics and multi-material **tritium transport** with **FESTIM** [1] and **FEniCS** [2]



Accurately **evaluate tritium inventory** in structural materials

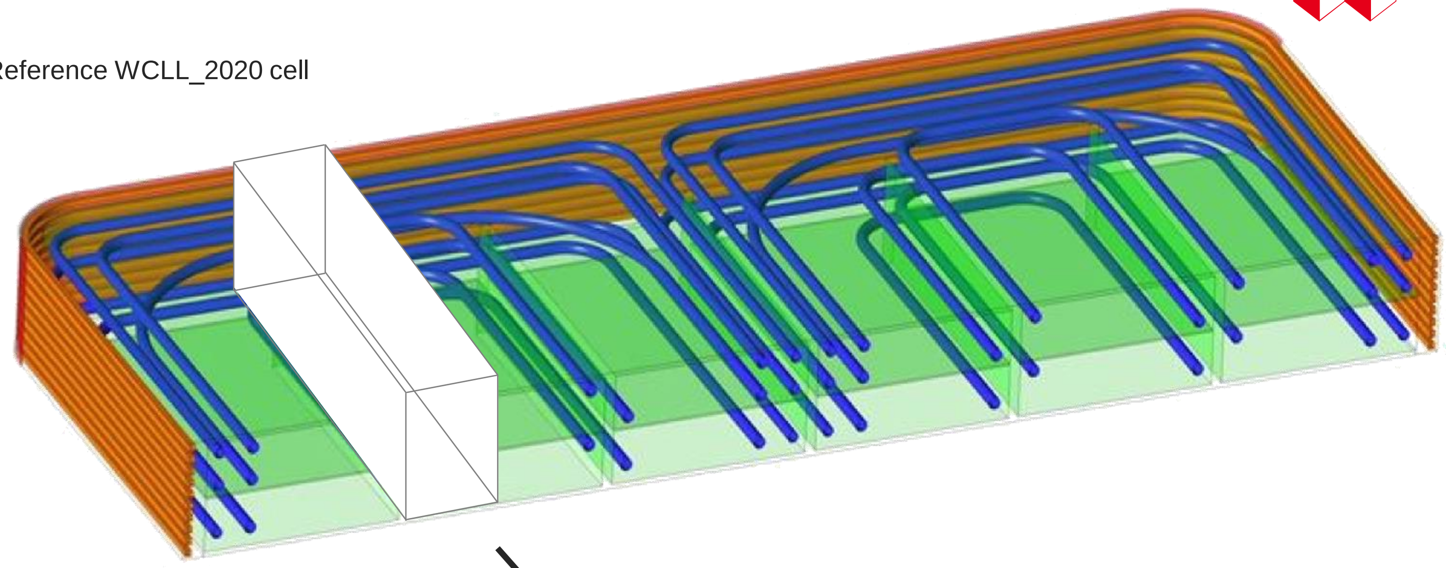
Evaluate tritium permeation to cooling channels

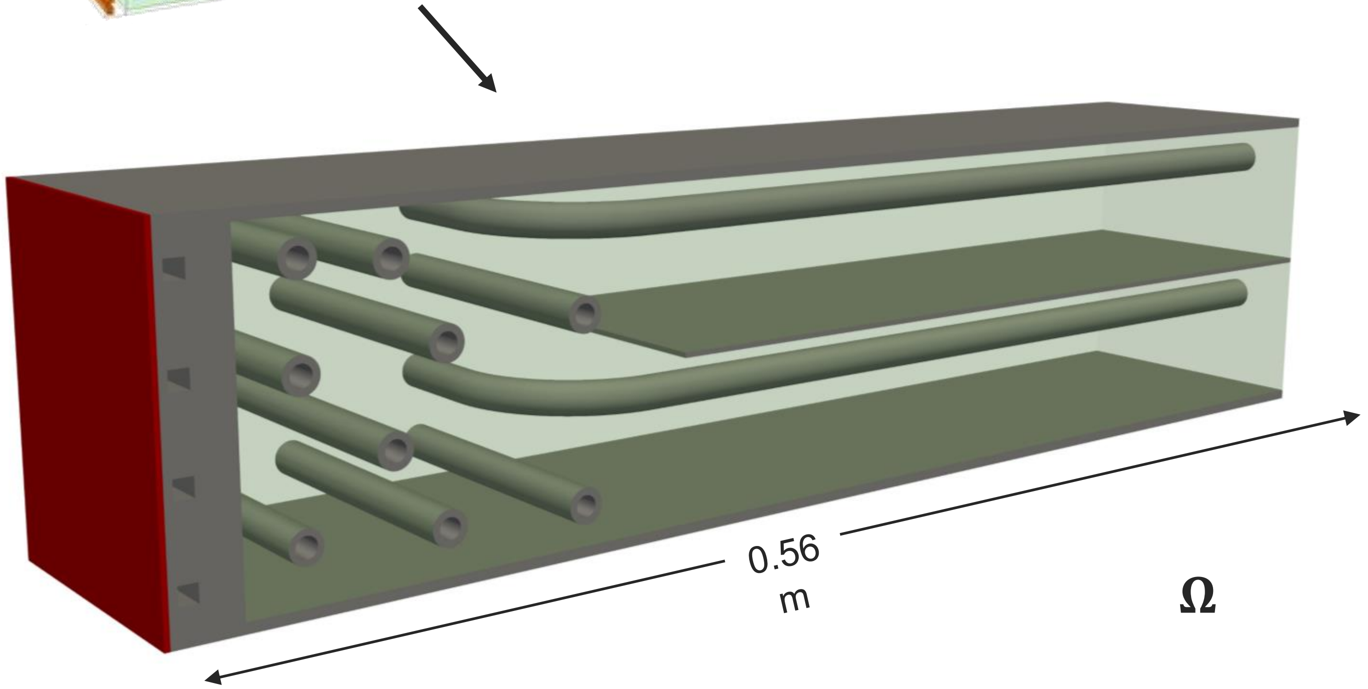


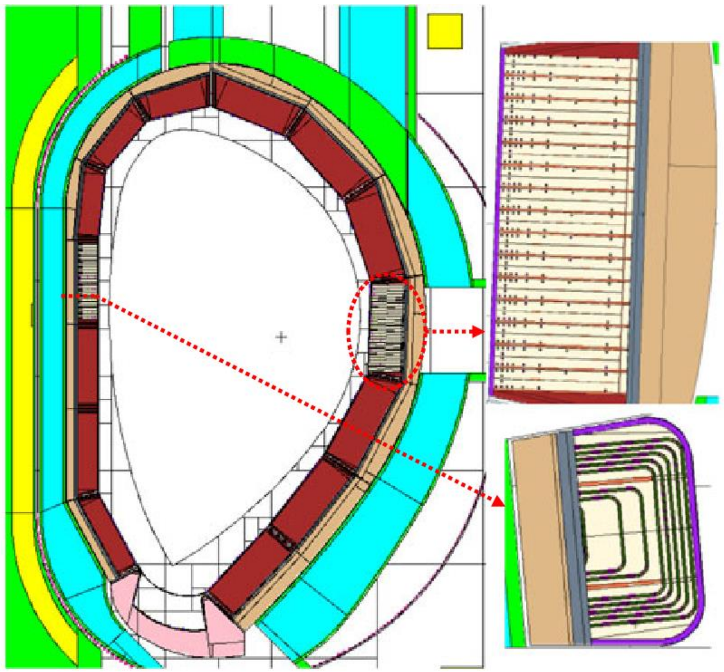
[1] - Delaporte-Mathurin *et al,* NME (2019)
[2] - Alnaes *et al,* Archive of Numerical Software (2015)

Geometry WCLL

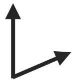
Reference WCLL_2020 cell





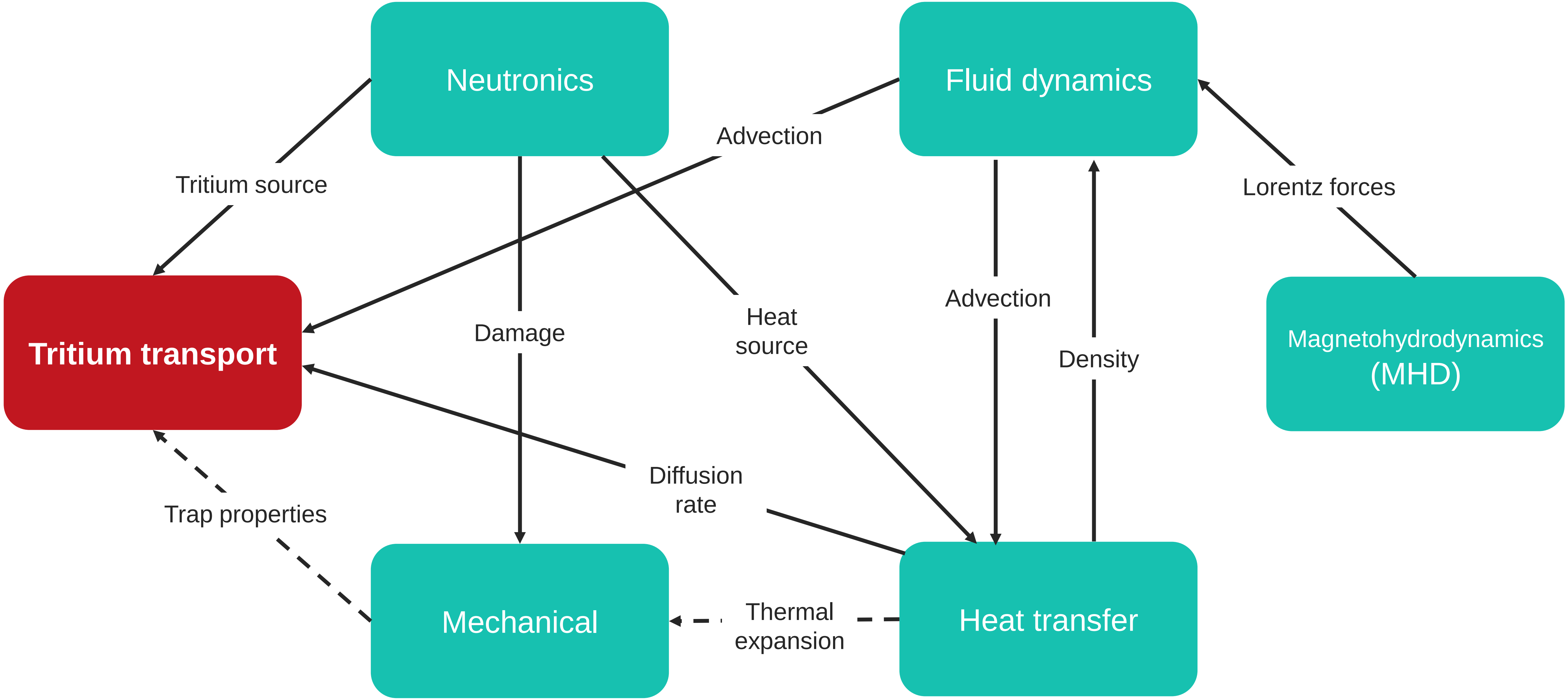


DEMO cross section



Tungsten	(red)
Lithium Lead	(green)
EUROFER	(grey)

The Multiphysics Issue



Governing equations

FEniCS

Fluid dynamics

$$\rho(T)\frac{\partial \mathbf{u}}{\partial t} + \rho(T)(\mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \mu(T)\nabla^2\mathbf{u} - \rho\mathbf{g}\big(1-\beta(T-T_0)\big)$$ on Ω_{fluid}

$$\vec{\nabla}\cdot\mathbf{u} = 0$$ on Ω_{fluid}

FESTIM

Heat transfer

$$\rho c_p\frac{\partial T}{\partial t} = \rho c_p(\mathbf{u}\cdot\nabla)T + \nabla\cdot(\lambda\nabla T) + Q$$ on Ω

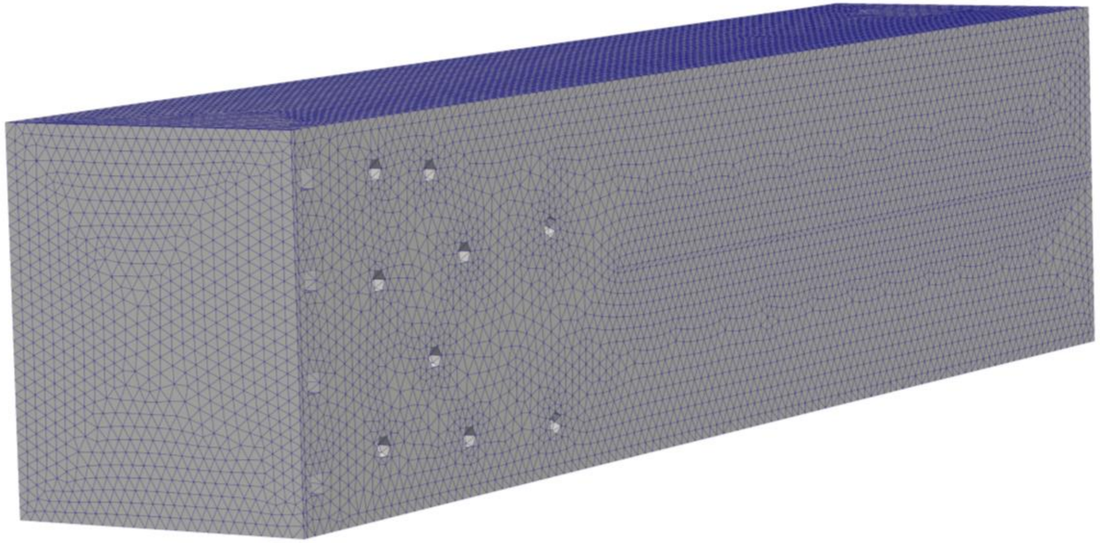
Tritium transport

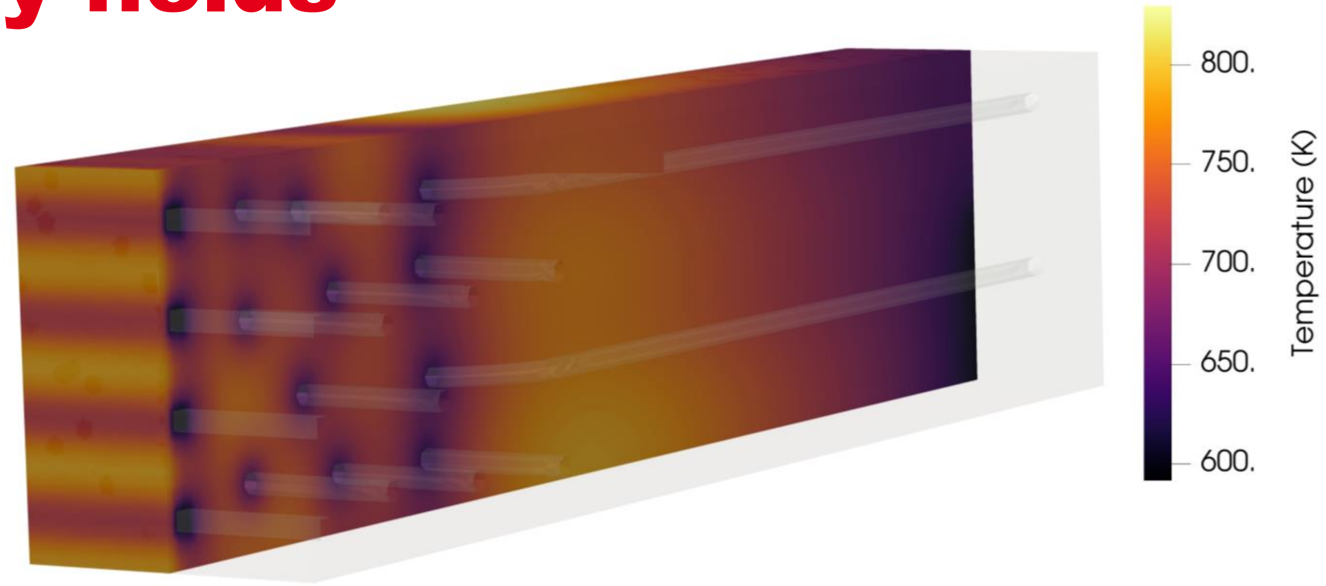
$$\frac{\partial c_{\mathrm{m}}}{\partial t} = \nabla\cdot(D(T)\cdot\nabla c_{\mathrm{m}}) + S + \mathbf{u}\nabla c_{\mathrm{m}} - \sum\frac{\partial c_{\mathrm{t},i}}{\partial t}$$ on Ω

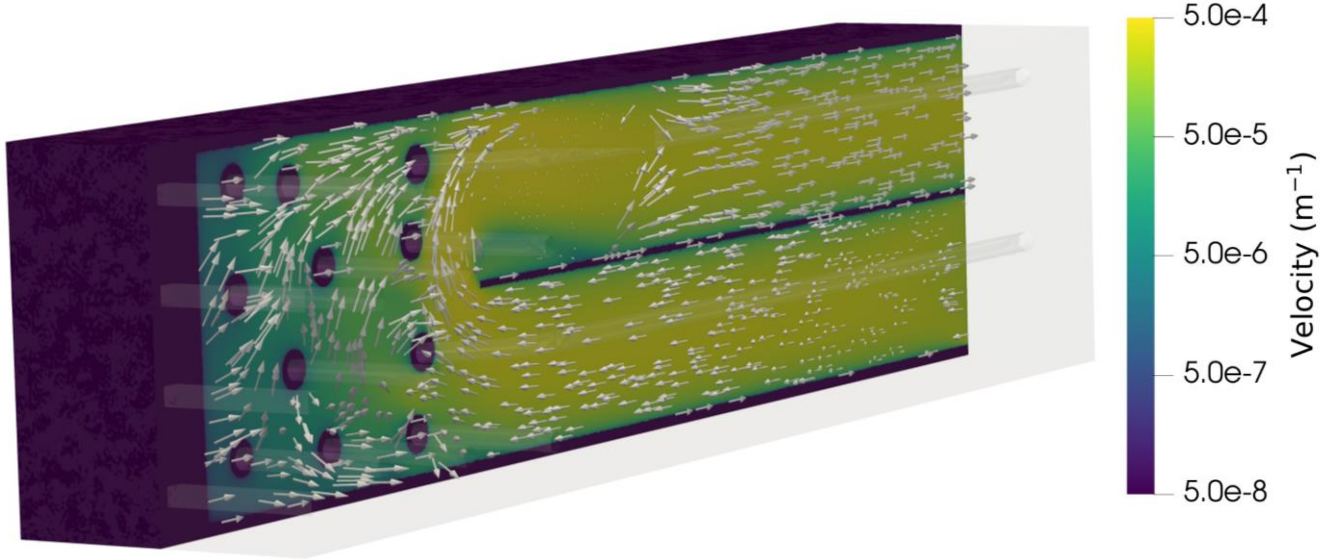
$$\frac{\partial c_{\mathrm{t},i}}{\partial t} = \nu_{t,i}(T)\cdot c_{\mathrm{m}}\cdot\big(n_i - c_{\mathrm{t},i}\big) - \nu_{dt,i}(T)\cdot c_{\mathrm{t},i}$$ on Ω_{solid}

McNabb & Foster – Trans. Metal. Soc. (1963)

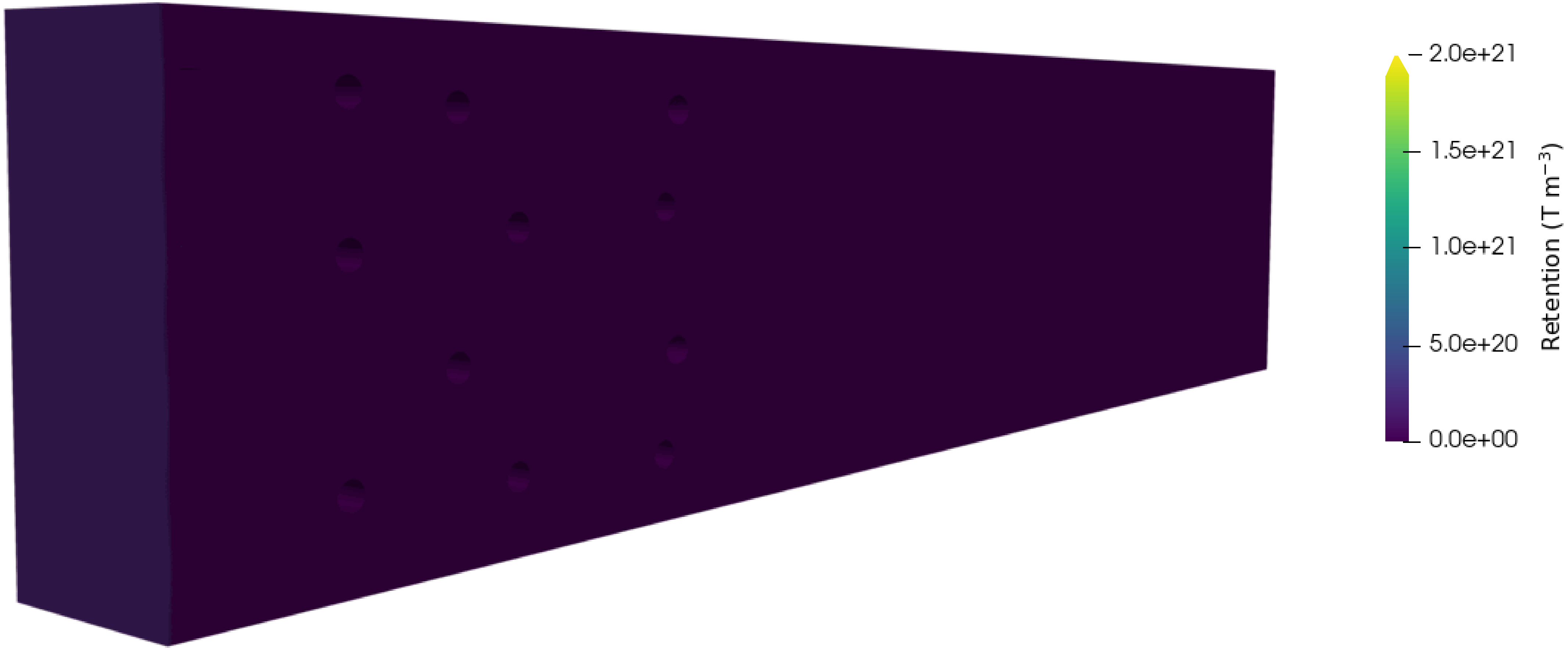
Temperature & velocity fields







Tritium transport



- 2D WCLL model: traps increased inventories by 15 % [1]

Inventories [g/tonne]	
Eurofer	1.25×10^{-2}
Tungsten	2.69×10^{-4}

Cooling ch. Flux [g/m2/s]	
First Wall	9.8×10^{-5}
Breeding Zone	1.5×10^{-4}

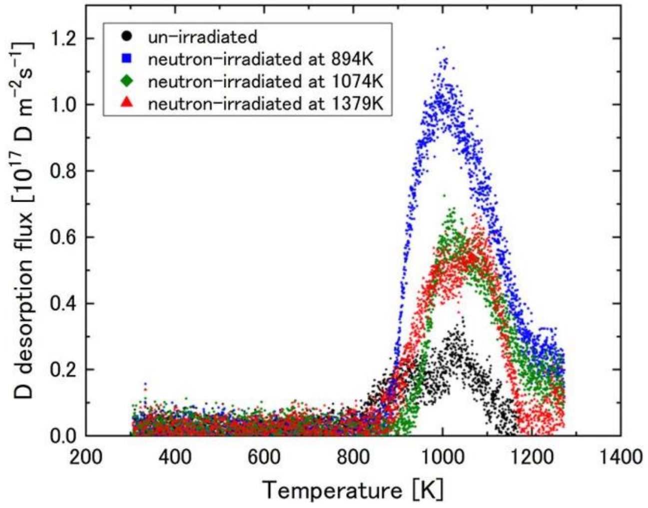
[1] - Dark *et al*, Nuc Fusion (2021)

Influence of neutron damage

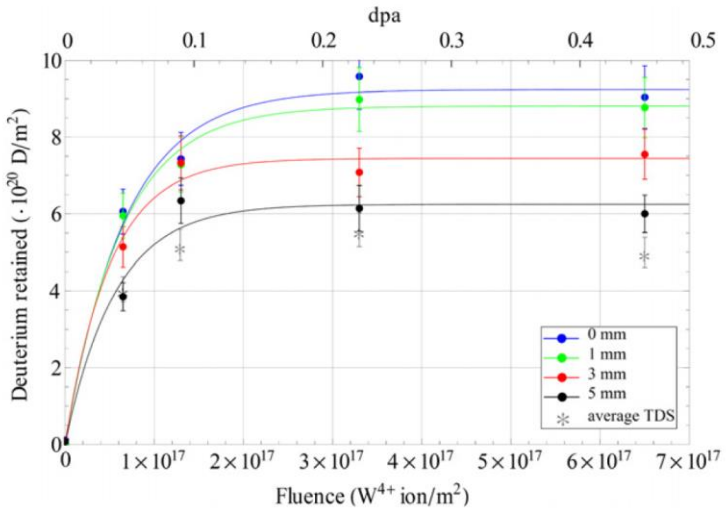
How will neutron damage influence tritium transport?

Influence of neutron damage

- Neutron damage will induce defects in structural materials
- Literature shows temperature dependence and saturation in D retention
- Traps reflect the microstructural defect landscape
  - Neutron damage will change this landscape
  - So must the traps used to model them



Desorption data from damaged tungsten samples [1]



Deuterium retention saturation with damage [2]

[1] - Tyburska *et al*, JNM (2009) [2] - Hoen *et al*, Nuc Fusion (2011)

Damage induced traps

Creation from damage − Destruction by annealing

$$\frac{\partial n_t}{dt} = \phi \cdot K \left[1 - \frac{n_t}{n_{\max,\phi}}\right] - A \cdot n_t$$

trap density [m^{-3}]

damage rate [dpa s^{-1}]

trap creation factor [m^{-3} dpa^{-1}]

maximum trap density [m^{-3}]

trap annealing factor [s^{-1}]

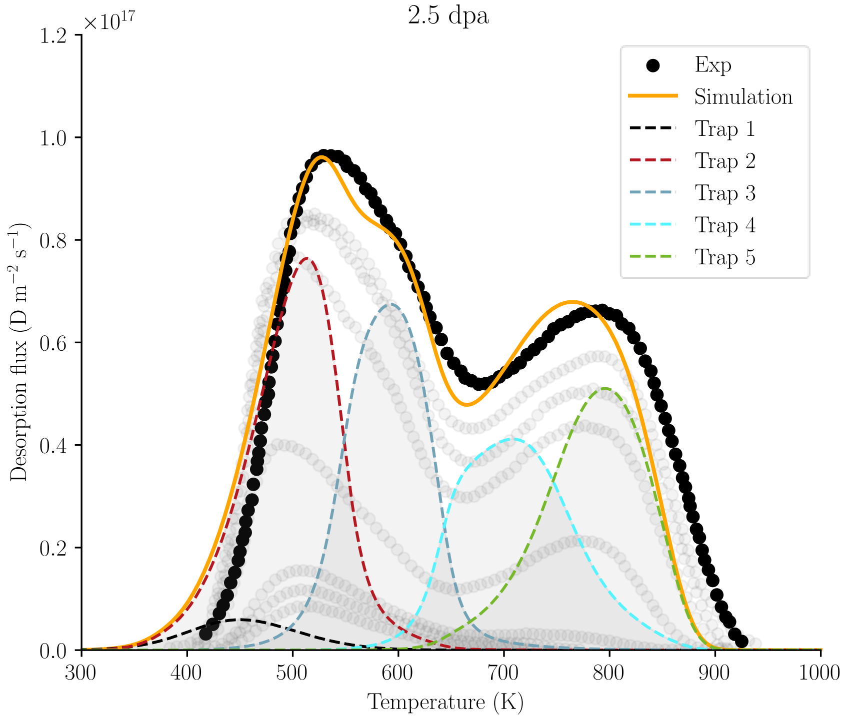
Assumptions

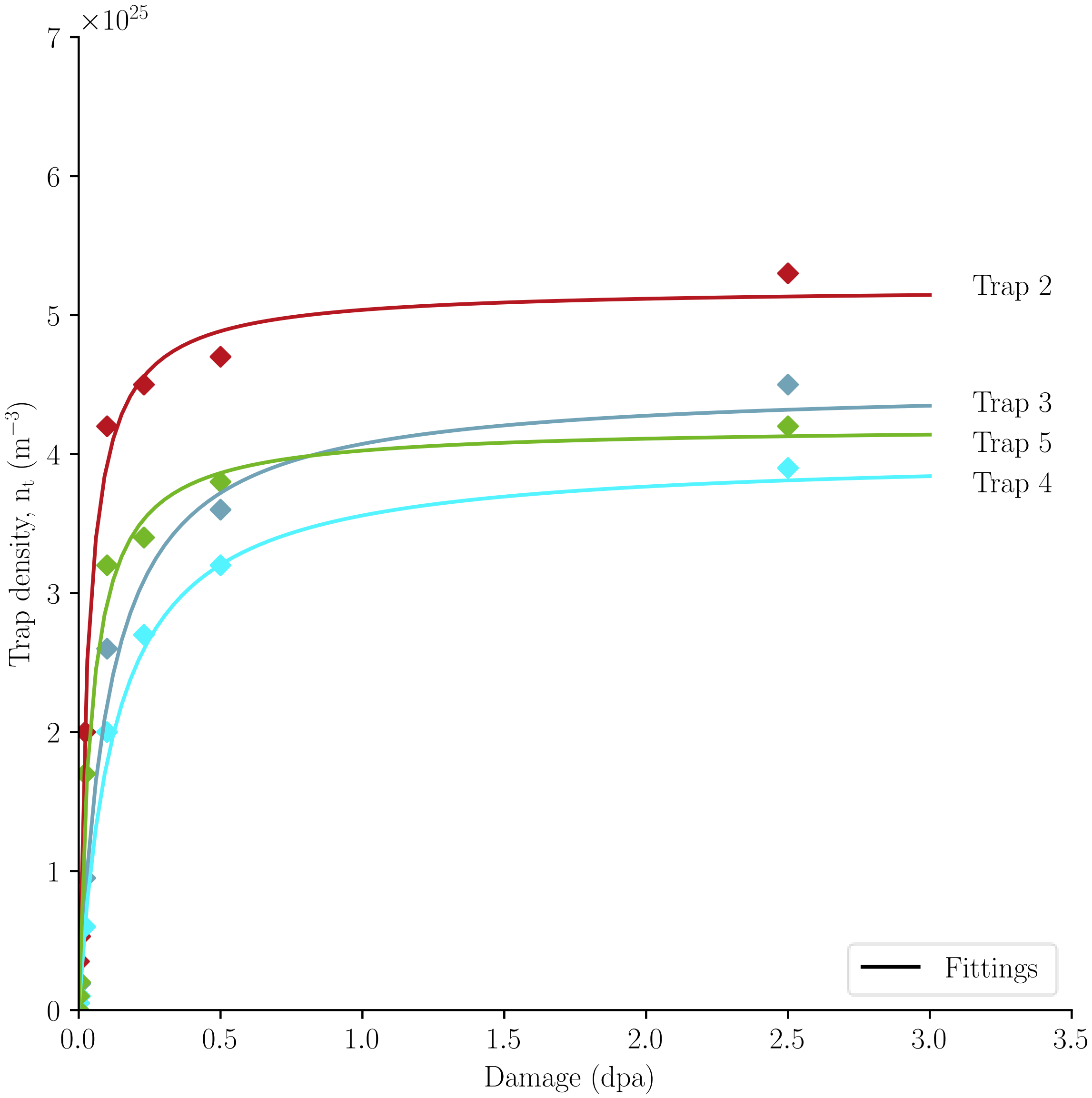
- Presence of hydrogen has no effect on trap creation
- Filled and empty traps have same annealing properties

Model parametrisation

Experiments conducted by T.Schwarz-Selinger

- Self-damaged W samples used in TDS experiments fitted with extrinsic traps
- Trap density evolution fitted using current model





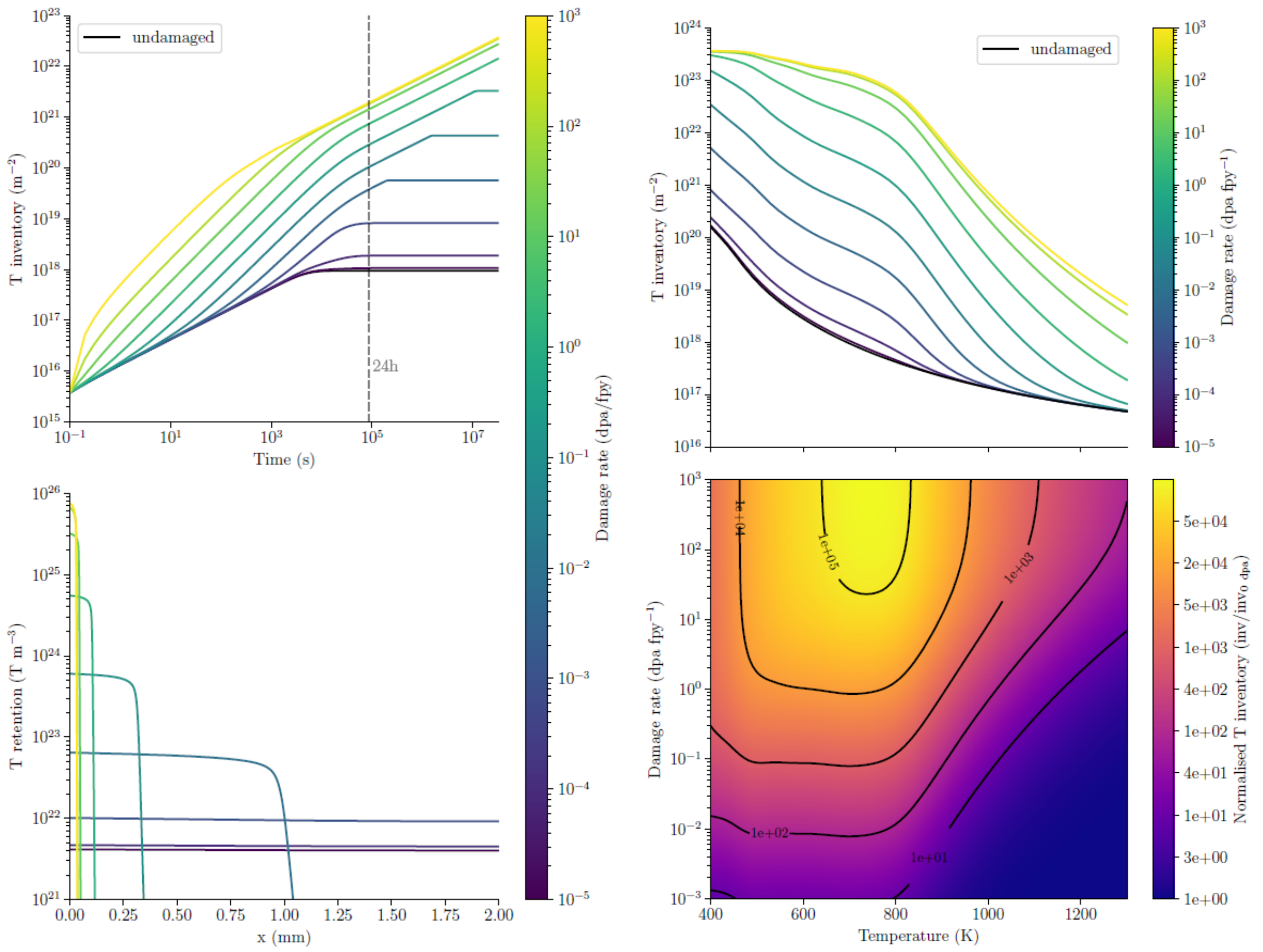
Influence of damage

<u>Case (FW conditions)</u>

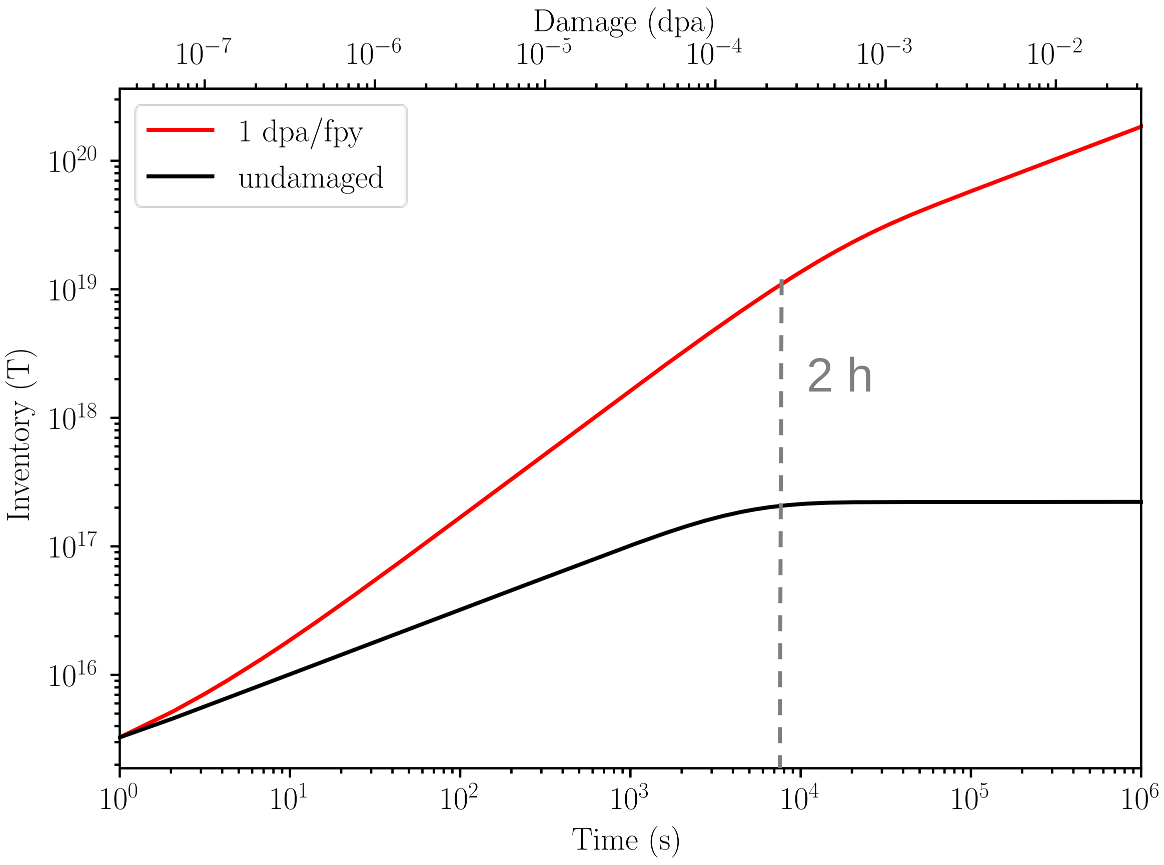
- 1D model of 2mm tungsten
- Implantation source and reflective BC's
- 400-1300 K and 10^{-5} to 10^{3} dpa/fpy

- At 24h, inventory increased by 3 orders of magnitude
- Steady-state inventories can increase beyond 5 orders of magnitude

- Work has been submitted to NME, with accompanying GitHub repo [1]



Damaged WCLL case

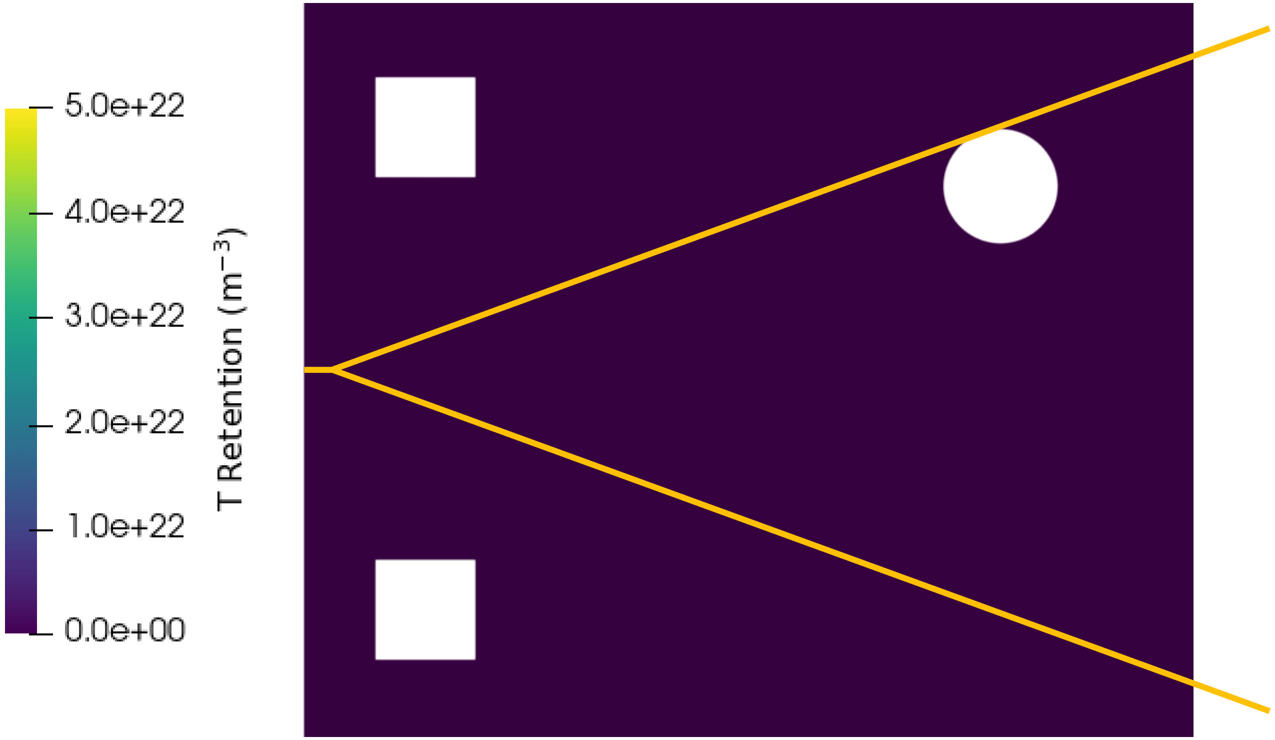


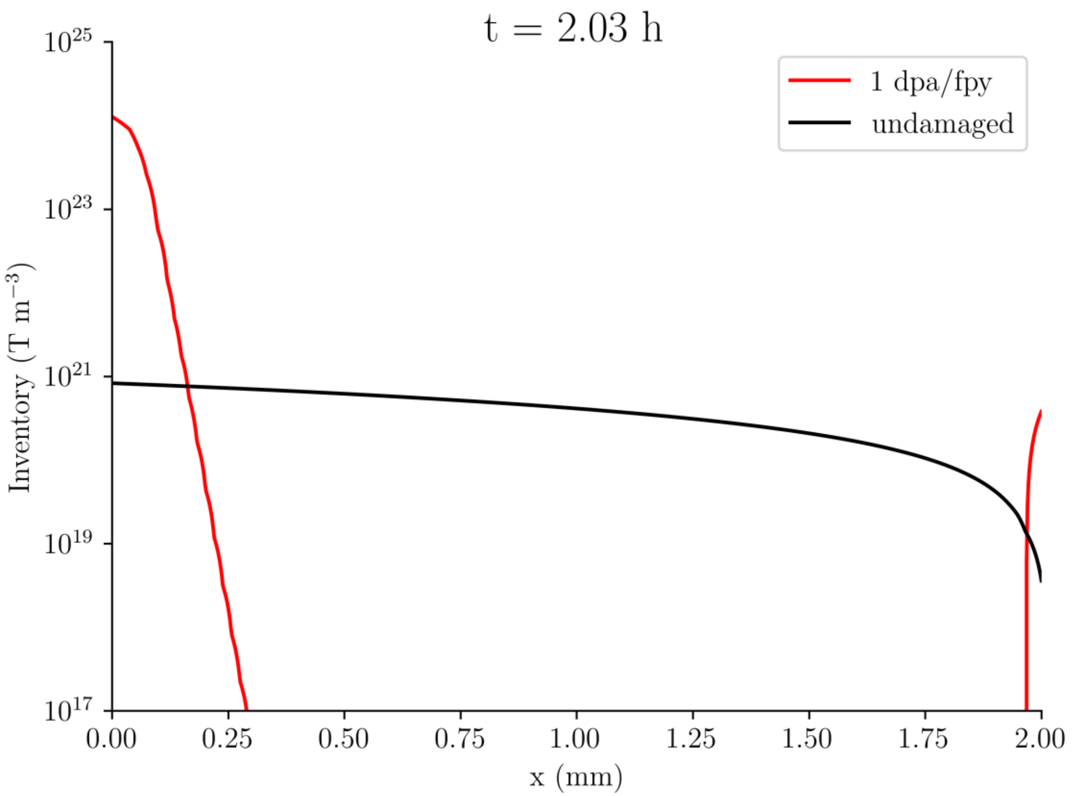
- WCLL simulations ran with damaged induced traps in tungsten FW

- Damage traps **increase** inventories by **50 X** after 2h
- **Increase** inventories by **700 X** after 11 days

Damaged WCLL case

Retention fields in WCLL



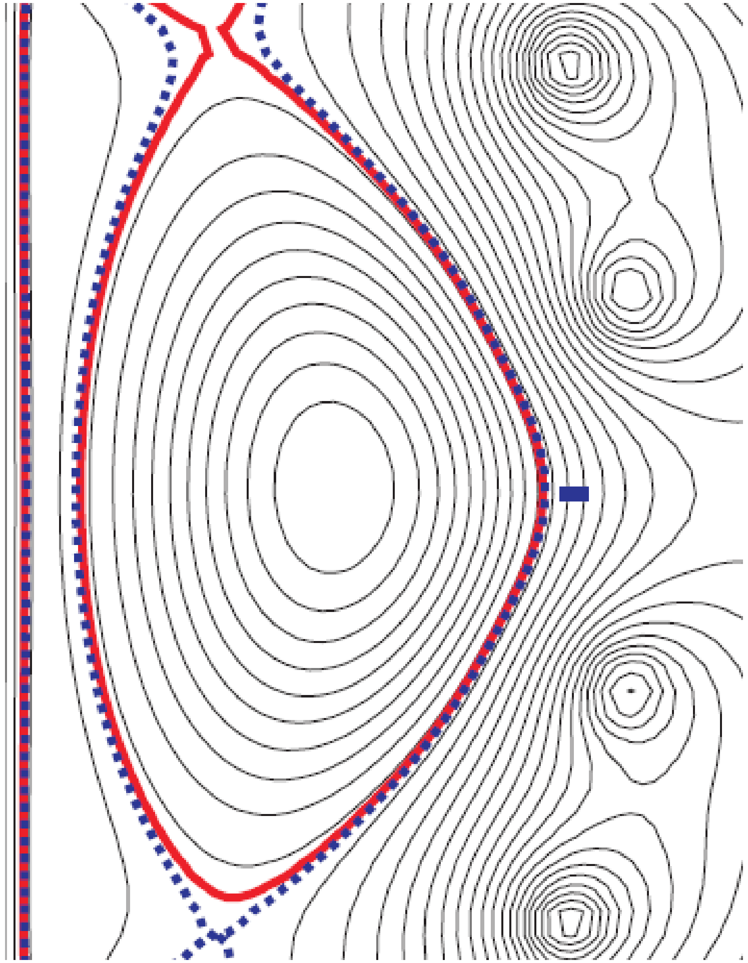


After 2h inventory contained within 0.3mm

Influence of MHD effects

How will the presence of a strong magnetic field affect tritium transport?

Influence of MHD effects

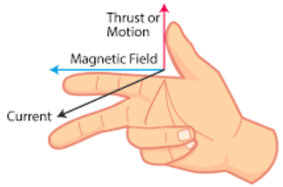


Poloidal projection field lines MAST [1]

Movement of liquid metal in a magnetic field

→ Induces a current

→ Inducing a force on the liquid

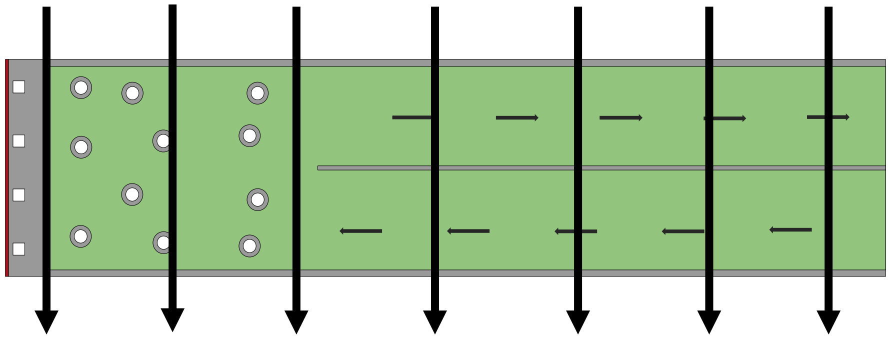


How will the presence of a magnetic field affect the flow of the PbLi breeder?

[1] - Hnat *et al*, Nuc. Fusion (2008)

MHD governing equations

$B = 4.0\ \mathrm{T}$



- Uniform magnetic field across domain
- Fluid dynamics equations need updating:

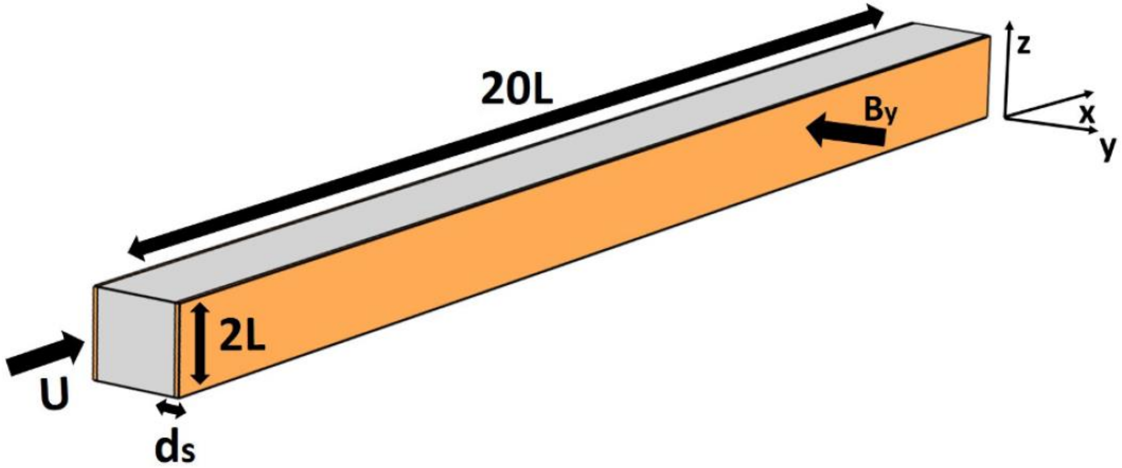
MHD

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho(\vec{u}\cdot\nabla\vec{u}) = -\nabla p + \mu\nabla^2\vec{u} - \rho\vec{g}\big(1-\beta(T-T_0)\big) + \vec{J}\times\vec{B}$$

$$\nabla\cdot\vec{u} = 0$$

$$\left.\begin{aligned} \nabla\cdot\vec{J} &= 0 \\ \vec{J} &= \sigma(-\nabla\phi + \vec{u}\times\vec{B}) \end{aligned}\right\} \quad \nabla^2\Phi = \nabla\cdot(\vec{u}\times\vec{B})$$

MHD benchmark



- Classic MHD benchmark [1]:

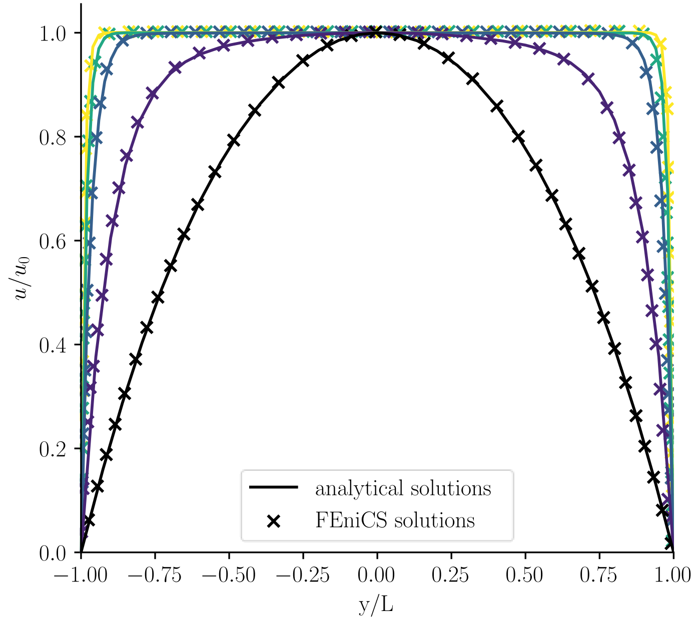
  Rectangular duct flow

- Testing Hartmann values:

  0 < Ha < 100

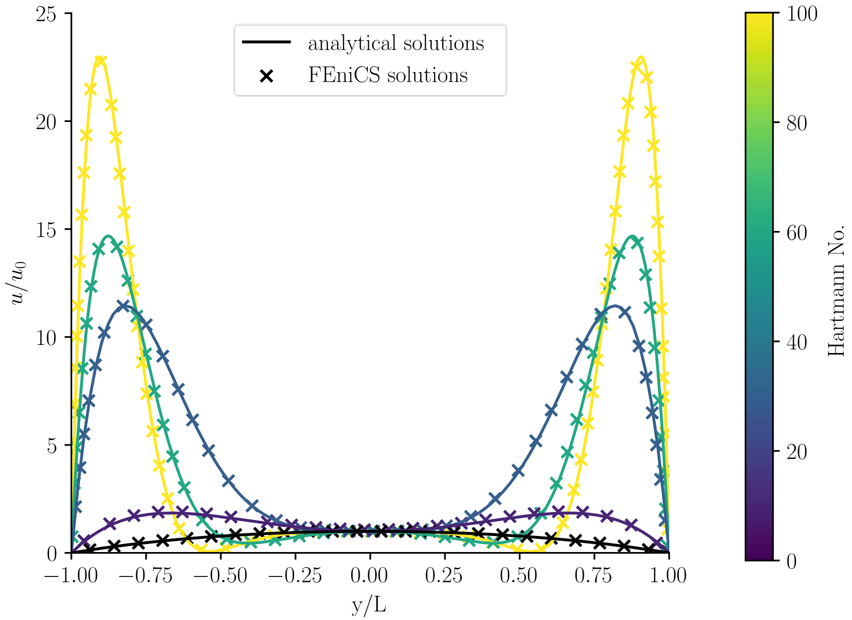
Fully insulated case [2]

$\left(\frac{\partial \phi}{\partial x} = 0 \quad \Gamma_{HW}\right)$



Fully conductive case [3]

$(\phi = 0 \quad \Gamma_{HW})$



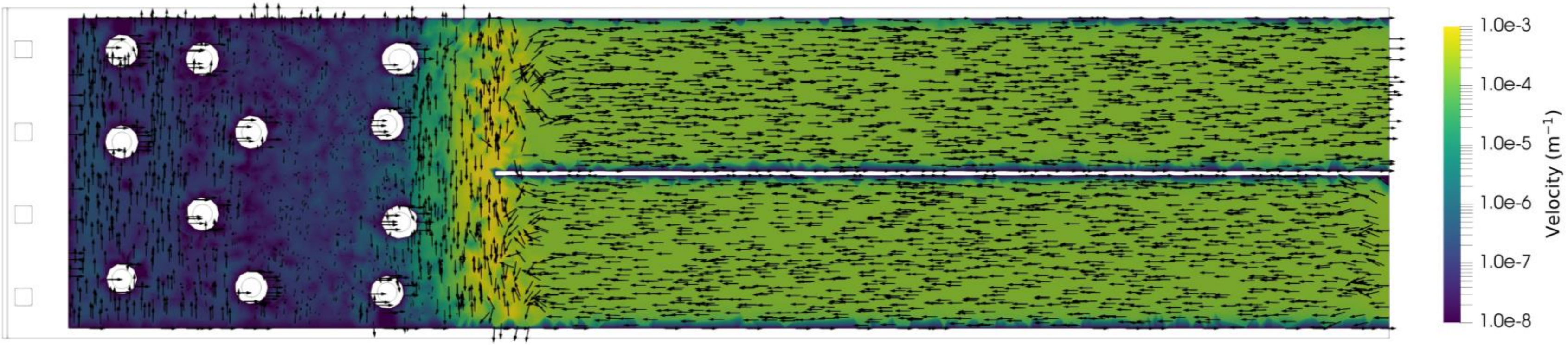
[1] - Blishchik *et al*, Int J Heat Fluid Flow (2021)

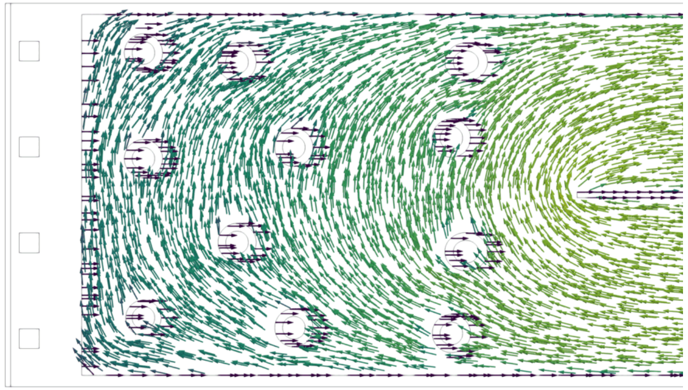
[2] - Shercliff, Math. Proc. Cambridge Philos. Soc. (1953)

[3] - Hunt, J. Fluid Mech. (1965)

WCLL case

- WCLL simulations not working perfectly yet
- Likely a numerical parameter or a mesh issue





Expected behaviour

- Increased velocities closest to the electrically conductive walls
  - ➢ Mitigating tritium diffusion into structure
    - ➢ Reducing permeation and tritium inventories

Conclusions and perspectives

Conclusions

- FEniCS and FESTM have been used to model tritium transport in a WCLL
- Damage induced traps will significantly increase tritium inventories
  - 50 x after 2 hours exposure
  - 700 X after 11 days exposure
- MHD effects work in progress

Perspectives

- Investigate influence of MHD forces on liquid metal flow in WCLL
- Investigate influence of neutron damage on trapping sites in Eurofer
- Model a specific DEMO plasma scenario
- Model permeation barriers

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Acknowledgement

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Backup slides

FESTIM

Starred 37

Features

- **F**inite **E**lement **S**imulation of **T**ritium **I**n **M**aterials
- Based on FEniCS
- 1/2/3D
- Multi-material
- Open-Source (apache 2.0)

Code	Dimensions	Heat transfer	Open Source	Programming Language
MHIMS	1D			Fortran
TMAP7	1D	✓		Fortran
HIT	1/2/3D	✓		COMSOL interface
FESTIM	1/2/3D	✓	✓	Python

Development plans →

FESTIMx

- Upgrade to FEniCSx (Oct – Nov)
- Update method for managing discontinuities at interfaces (DG methods)
- Create wrappers for OpenMC and other codes

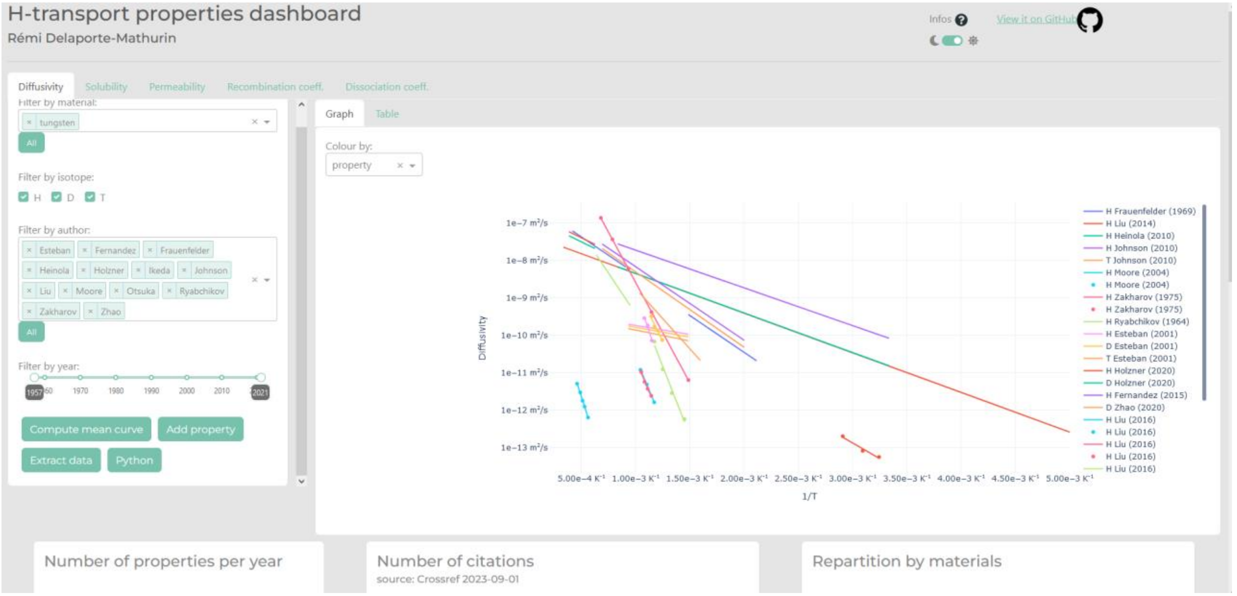
HTM

Starred 10

Features

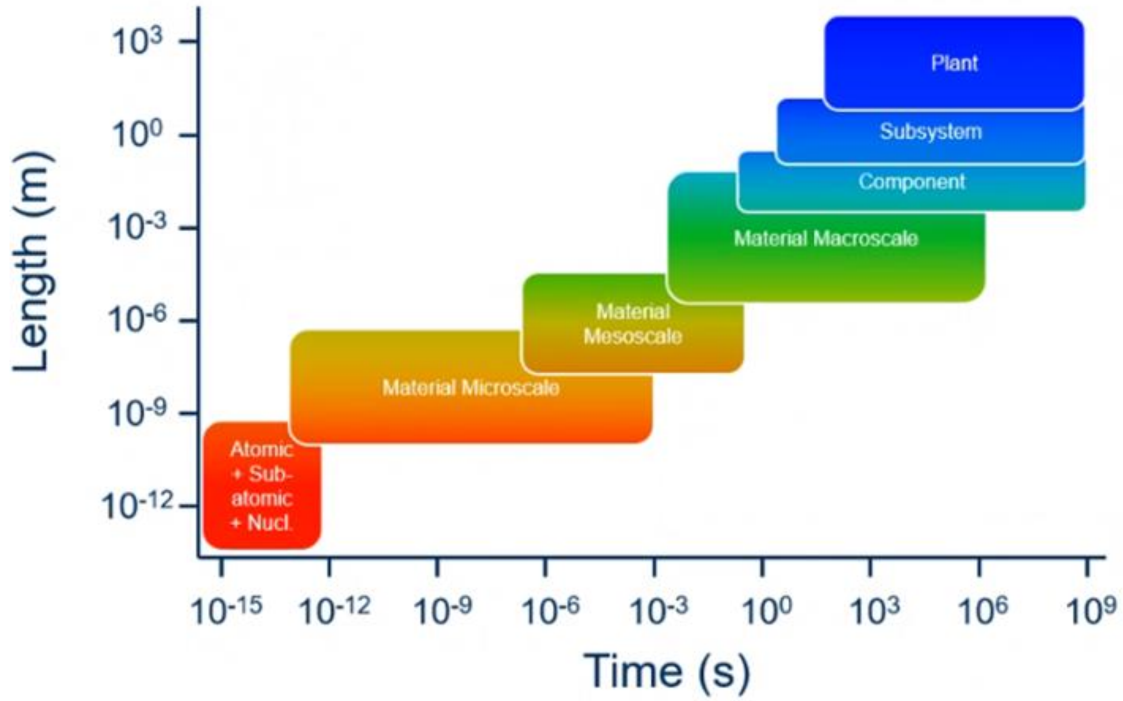
- **H**ydrogen **T**ransport **M**aterials
- Comprehensive database
- Accountable and transparent
- 400 + entries so far
- 40 materials
- Open-Source (MIT)

Online dashboard



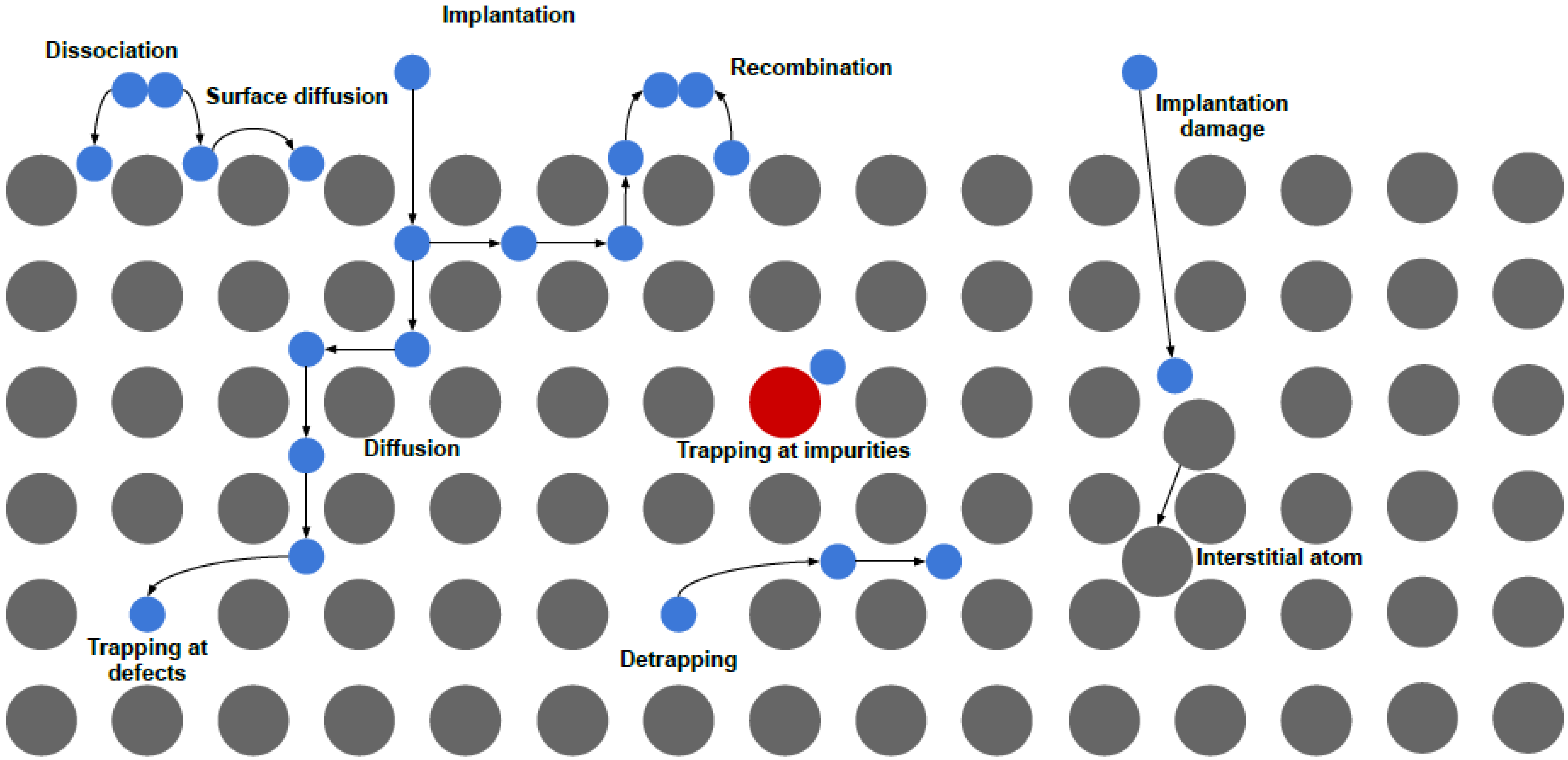
Recently highlighted on Plotly's Explore page!

Tritium transport overview



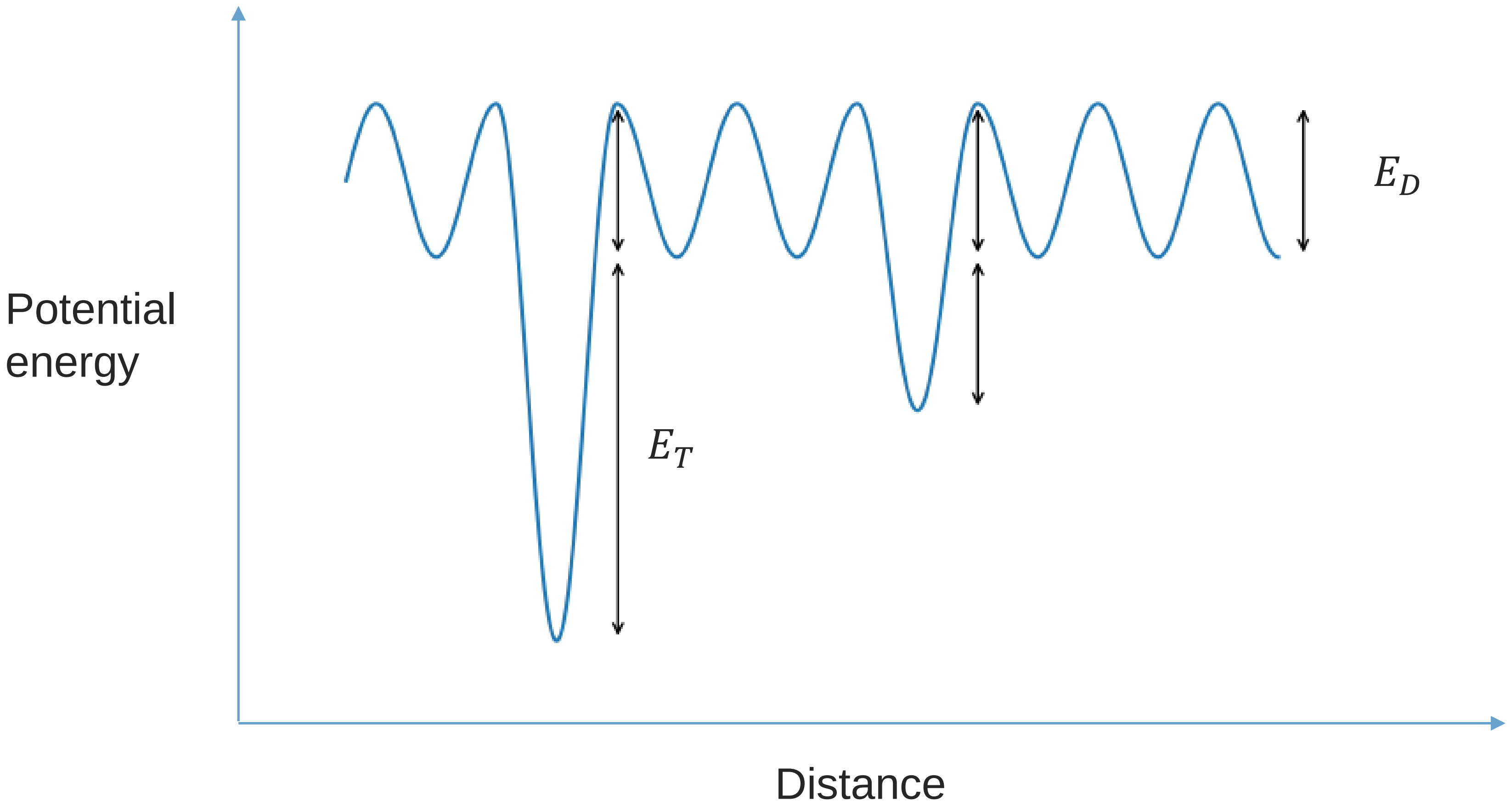
Model scale	What is considered	Models
Plant	operating conditions: temperatures, flows, partial pressures, mass balance	ASPEN, AVEVA
Subsystem	spatial configuration, component interaction, loss factors	ASPEN, AVEVA
Component	shape, function, gradients, loads	MNCP, TESSIM, TMAP, EcosimPro
Material Macro	phase distribution, grain size distribution, grain and phase boundaries, texture, long range stress fields	Transport phenomena
Material Meso	grain interactions, distribution of slip, interface effects, intragranular stress fields, fracture mode	??? (CPFEM)
Material Micro	pores, dislocation substructure, segregation, short range stress fields	MD, CRA
Atomic scale	vacancies, interstitials, clustering, crystallography	MD, interatomic potentials
Sub atomic	electronic structure, binding energies of traps	DFT
Nuclear core	nuclear transmutation processes, particle interaction cross-sections	Fispact

Trapping

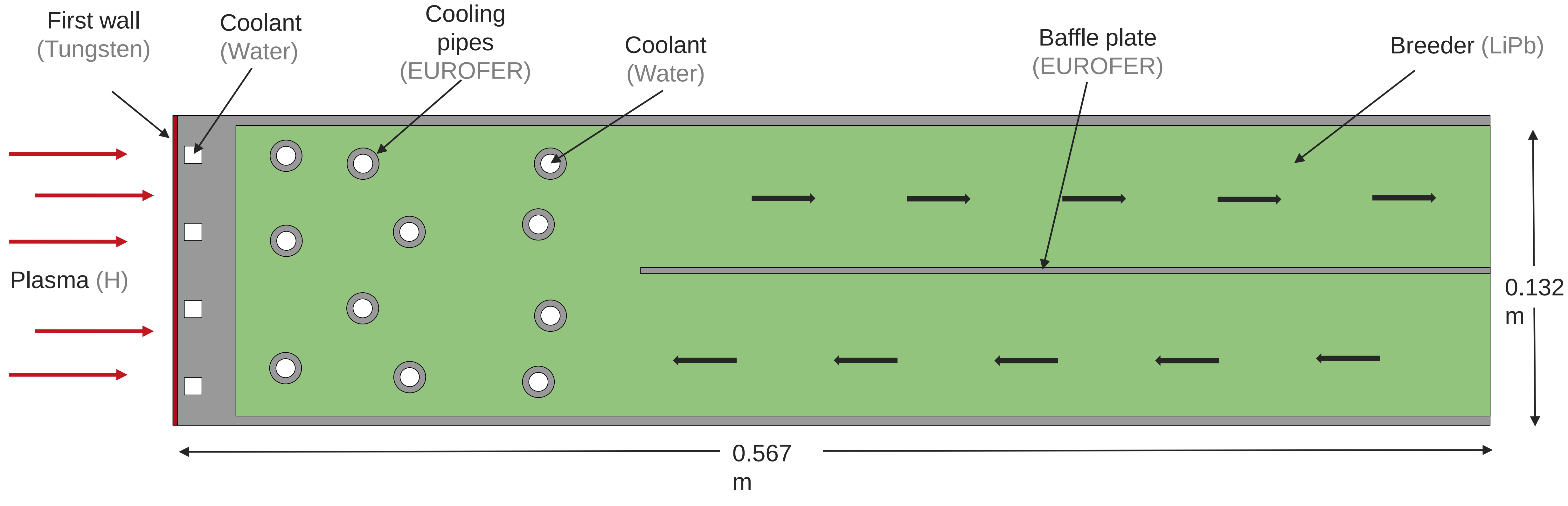


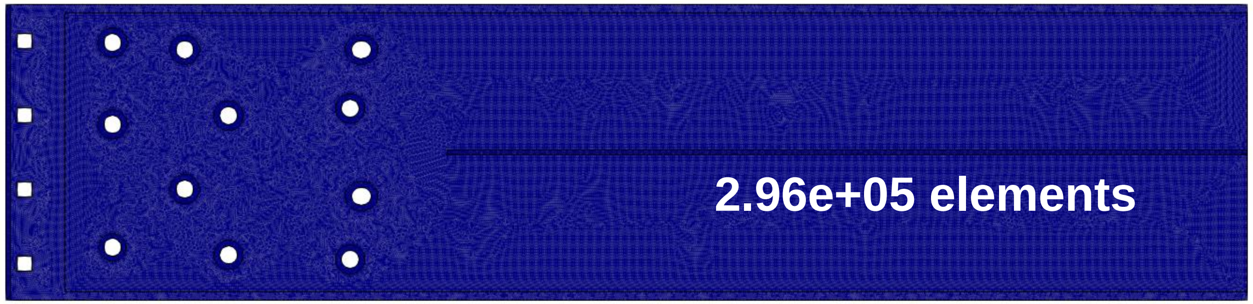
Implantation
Dissociation
Surface diffusion
Recombination
Implantation damage
Diffusion
Trapping at impurities
Interstitial atom
Trapping at defects
Detrapping

Trap modelling

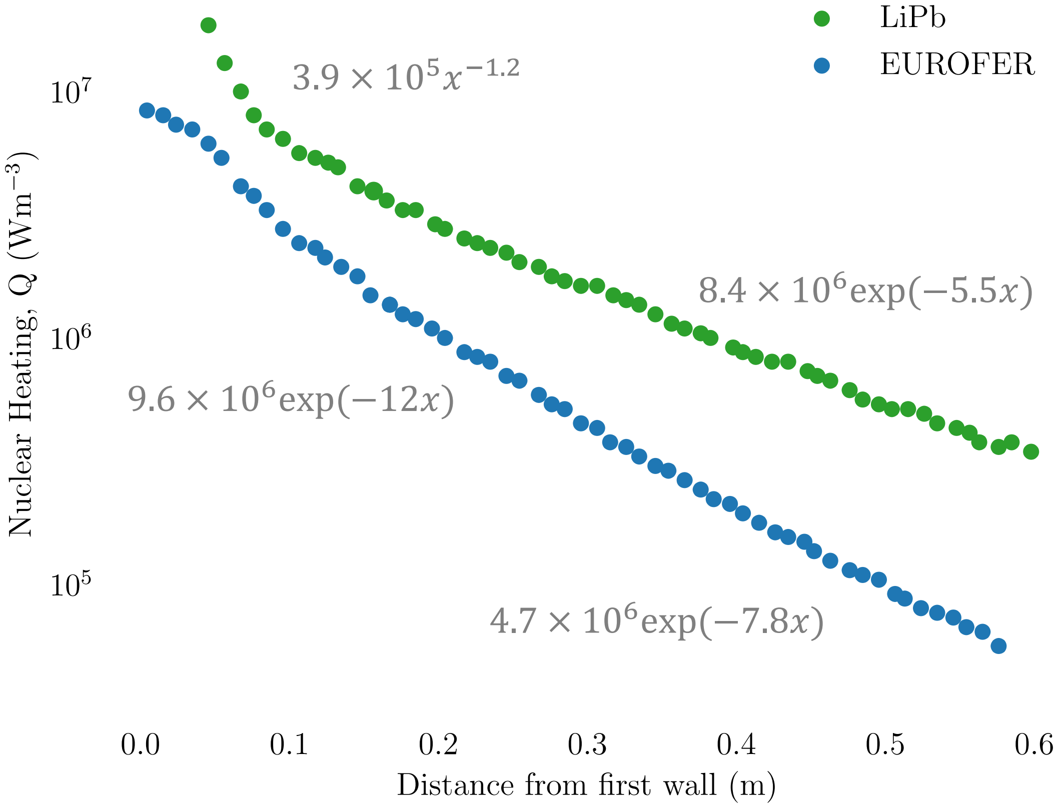


WCLL Geometry





Governing Equations – Source terms



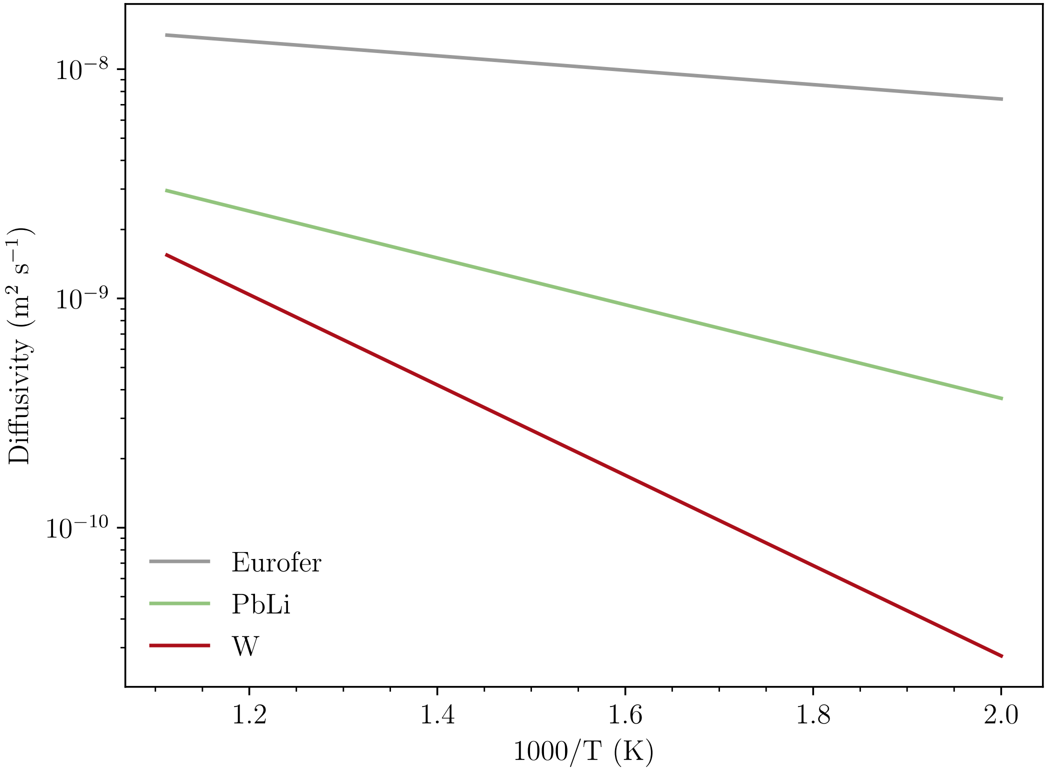
- Neutronics data for heat source [7]
- Fitted with decreasing exponential piecewise functions
- For W [8]:

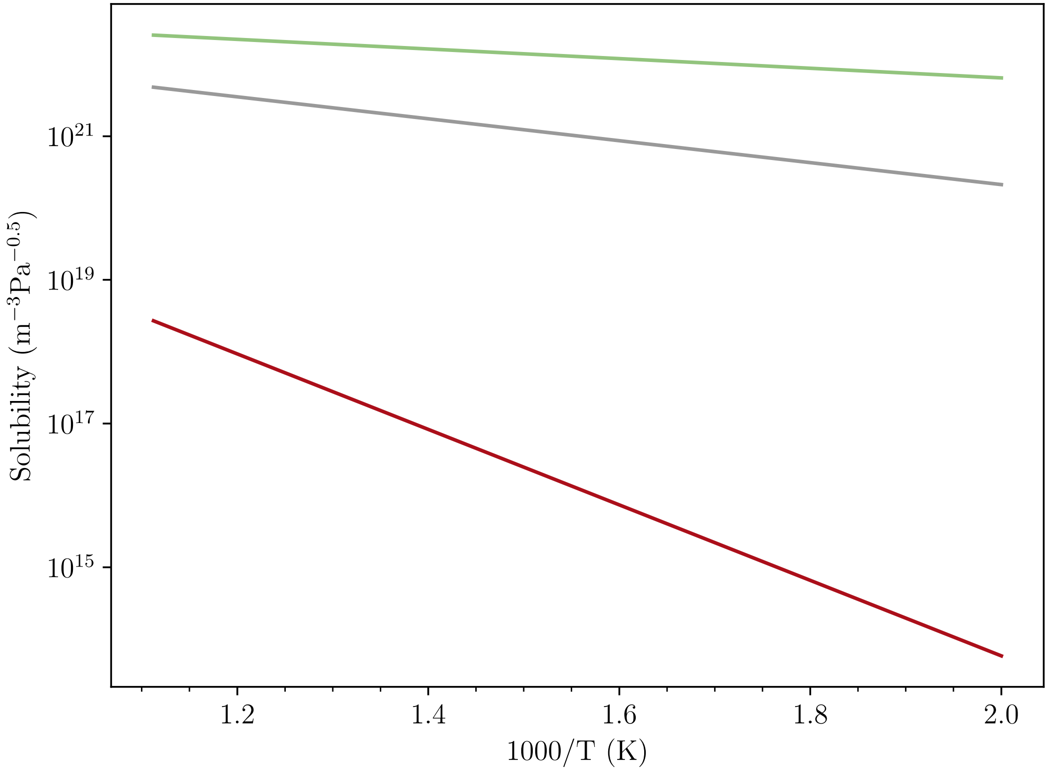
  $Q = 23.2 \exp(-71.74\, x)$ MW m^{-3}

- Tritium source term in LiPb [9]:

  $S = 5.59 \times 10^{18} \exp(-3.21\, x)$ $\mathrm{T\, m^{-3}\, s^{-1}}$

Hydrogen transport parameters





Properties from HTM

Material properties

Material	Trapping rate		Detrapping rate		Trap density
	k_0	E_k	p_0	E_p	n_i
Tungsten [5]	$5.22 \cdot 10^{-17}$	0.39	$1.00 \cdot 10^{13}$	0.87	$8.22 \cdot 10^{25}$
	$8.93 \cdot 10^{-17}$	0.39	$1.00 \cdot 10^{13}$	1.00	$2.53 \cdot 10^{25}$
EUROFER [10]	$2.53 \cdot 10^{-17}$	0.06	$1.00 \cdot 10^{13}$	0.78	$4.50 \cdot 10^{23}$
	$[\mathrm{m^3 s^{-1}}]$	$[\mathrm{eV}]$	$[\mathrm{s^{-1}}]$	$[\mathrm{eV}]$	$[\mathrm{m^{-3}}]$

- Two traps in Tungsten and one trap in EUROFER

Properties from HTM

Boundary conditions – heat and fluid transport

Imposed fluxes

$$-\lambda\vec{\nabla}T\cdot\vec{n} = h\,(T - T_c)$$

(Coolant interfaces)

$$-\lambda\vec{\nabla}T\cdot\vec{n} = \varphi_0$$

(First wall)

Symetry

$$-\lambda\vec{\nabla}T\cdot\vec{n} = 0$$

(Bottom, top and z=0 of domain)

Imposed Values

$$T = T_0$$
$$\vec{u} = \vec{u}_0$$

(Inlet)

$$\vec{u} = (0,0,0)$$

(Fluid walls)

$$P = P_0$$

(outlet)

Parameter	Values	Units
$T_{c,FW}$	585.35	[K]
$T_{c,BZ}$	584.9	[K]
h_{FW}	$2.23\cdot10^4$	$[\mathrm{W\,m^{-2}}K^{-1}]$
h_{BZ}	$1.59\cdot10^4$	$[\mathrm{W\,m^{-2}}K^{-1}]$
T_0	598.15	[K]
φ_0	0.5	$[\mathrm{MWm^{-2}}]$
u_{inlet}	0.2	$[\mathrm{mms^{-1}}]$
P_{outlet}	0	[Pa]

Boundary conditions – hydrogen transport

Recombination

$$-D\vec{\nabla}c_\mathrm{m} \cdot \vec{n} = K_r c_\mathrm{m}^2$$

(Coolant interfaces)

Symmetry

$$-\lambda\vec{\nabla}c_\mathrm{m} \cdot \vec{n} = 0$$

(Bottom and top of domain)

Implantation flux

$$c_\mathrm{m} = \frac{\varphi_\mathrm{imp}\, R_\mathrm{p}}{D}$$

(First Wall)

Conservation of chemical potential

$$\left(\frac{c_\mathrm{m}}{S}\right)_1 = \left(\frac{c_\mathrm{m}}{S}\right)_2$$

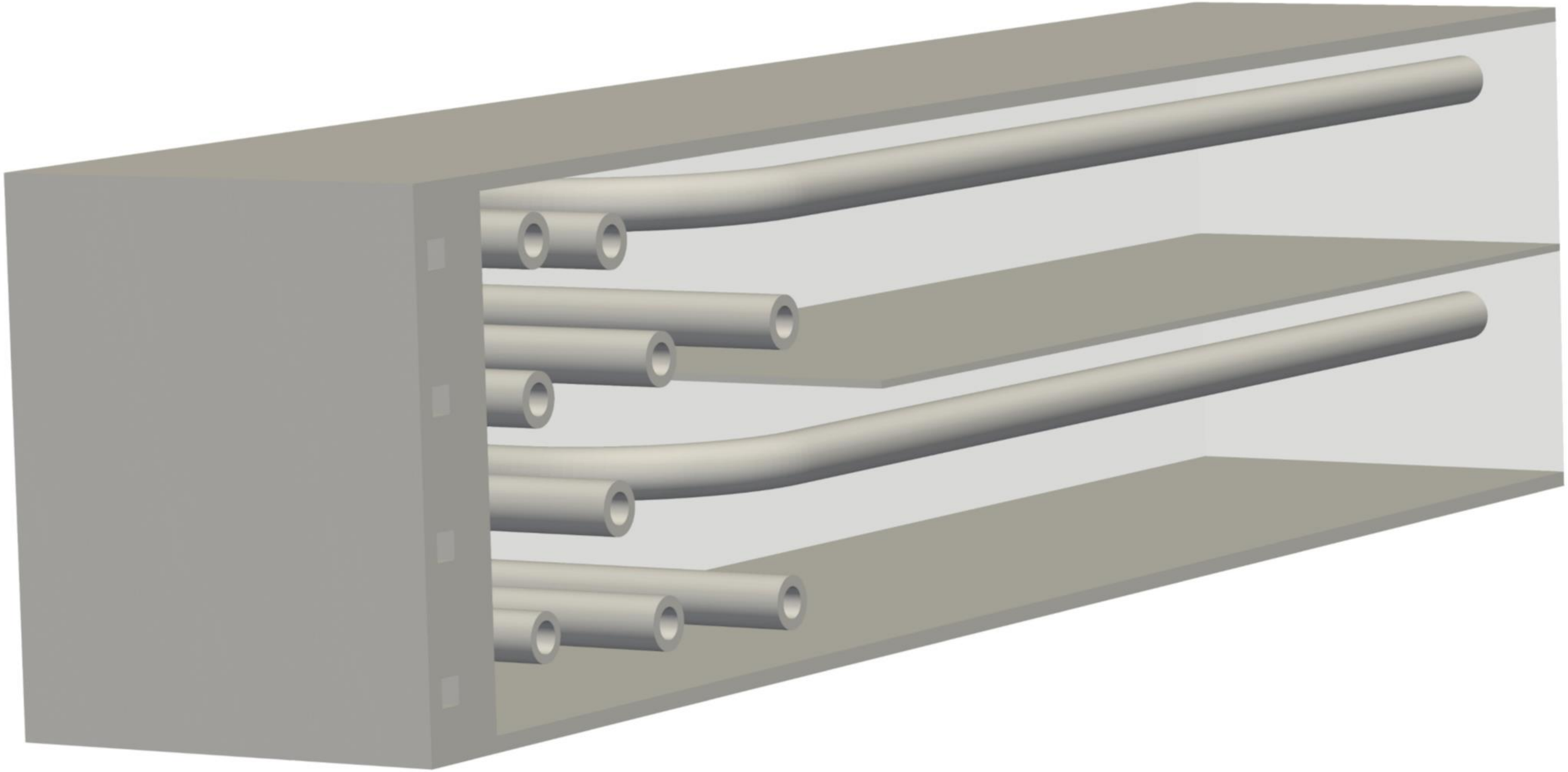
(All material interfaces)

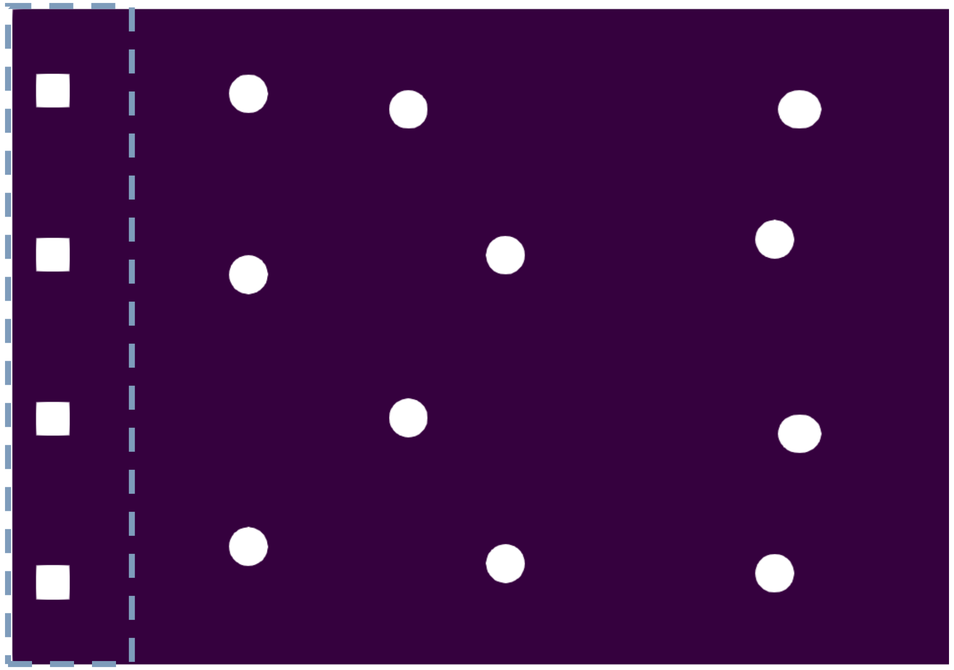
Values at 600k

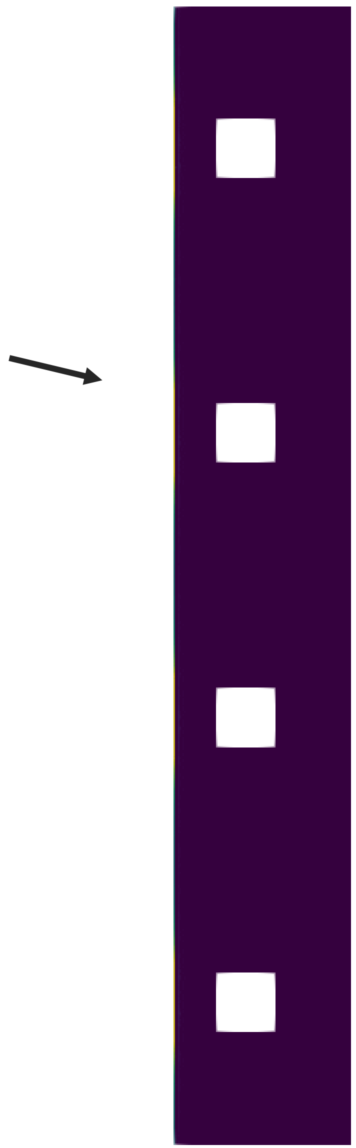
Parameter	Values	Units
φ_imp	10^{20}	$[\mathrm{m}^{-2}\mathrm{s}^{-1}]$
R_p	3	[nm]
K_r	$9.66 \cdot 10^{-29}$	$[\mathrm{m}^4\mathrm{s}^{-1}]$
$D_{EUROFER}$	$9.43 \cdot 10^{-9}$	$[\mathrm{m}^2\mathrm{s}^{-1}]$
D_W	$8.02 \cdot 10^{-10}$	$[\mathrm{m}^2\mathrm{s}^{-1}]$

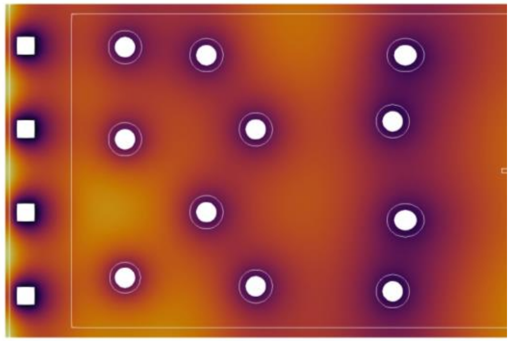
Properties from HTM

Model

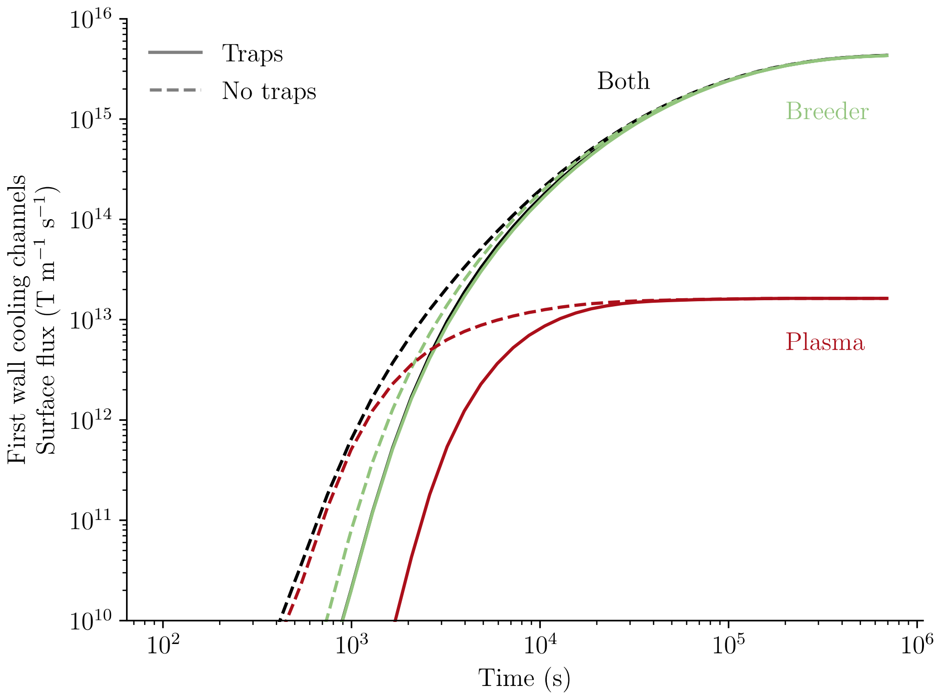


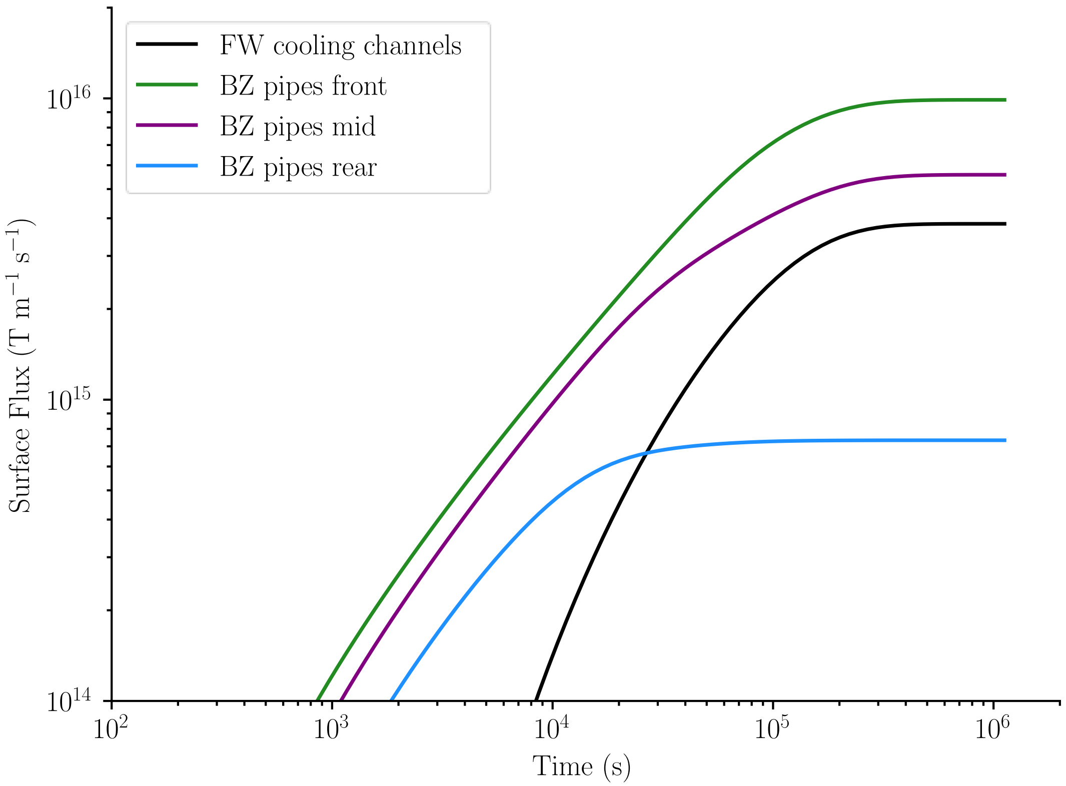


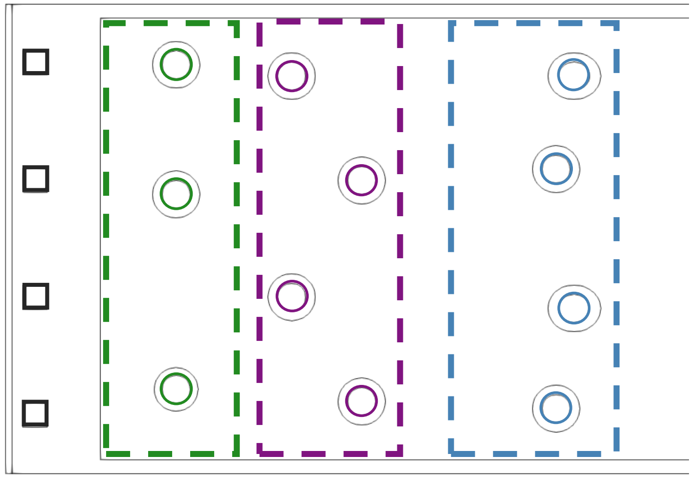


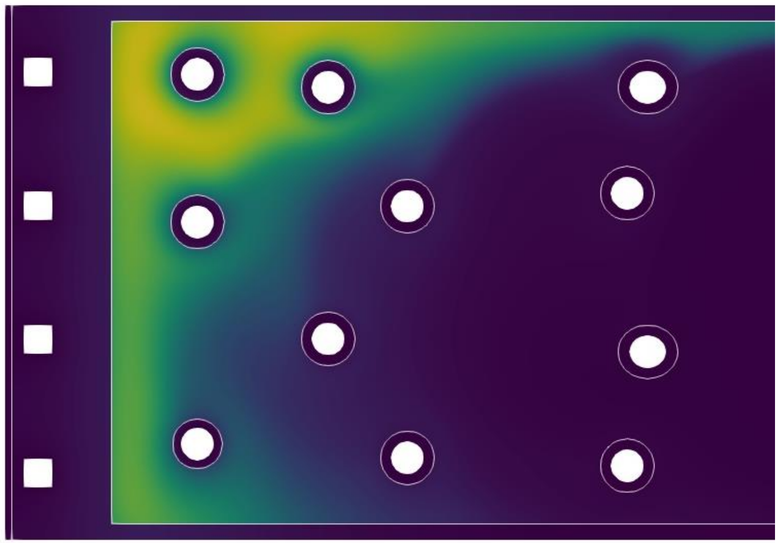


- **Larger contribution from LiPb breeder** than implantation from the plasma
- **2D edge effects** near FW cooling channel



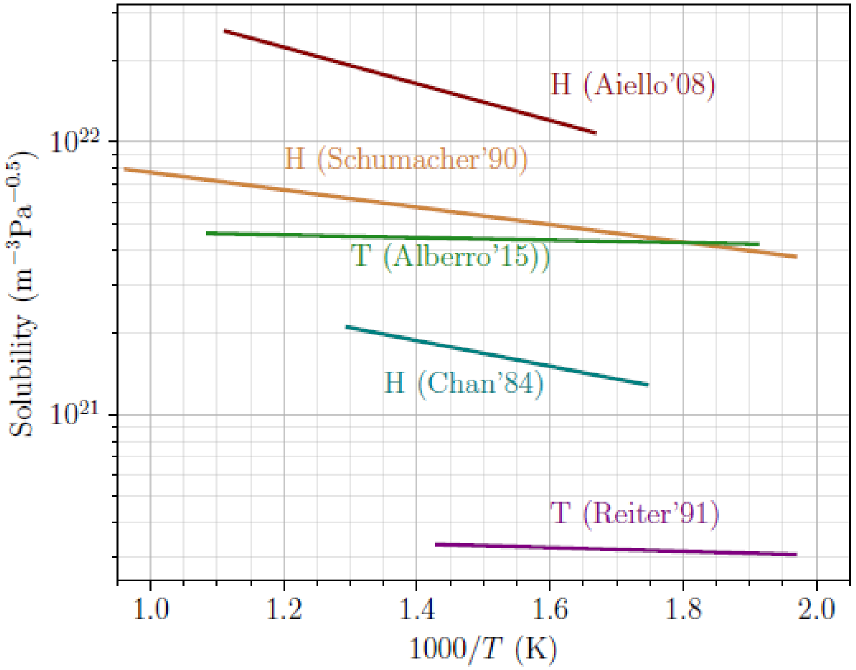


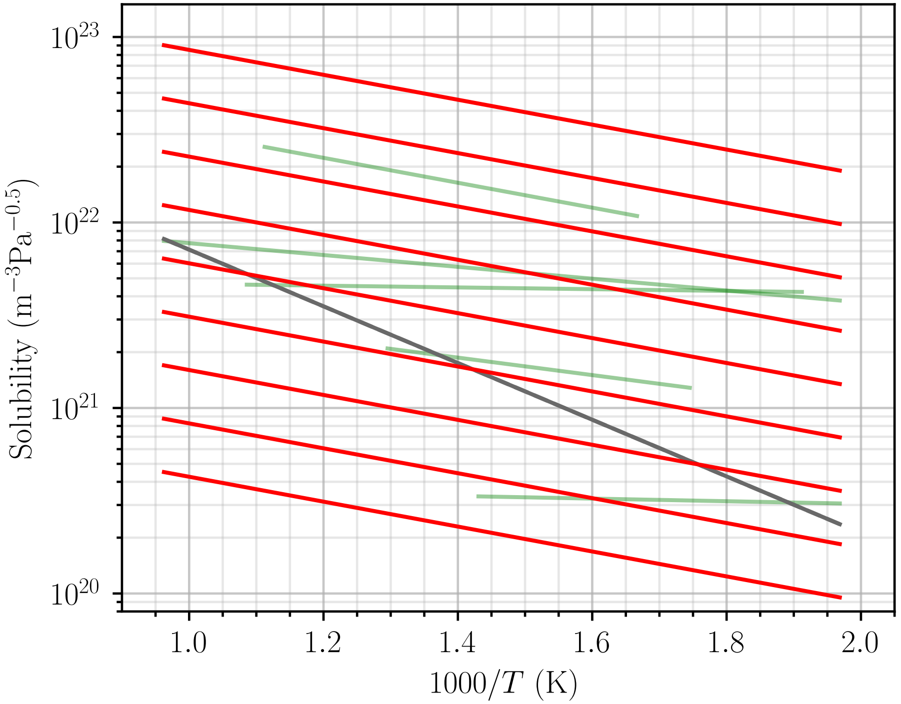




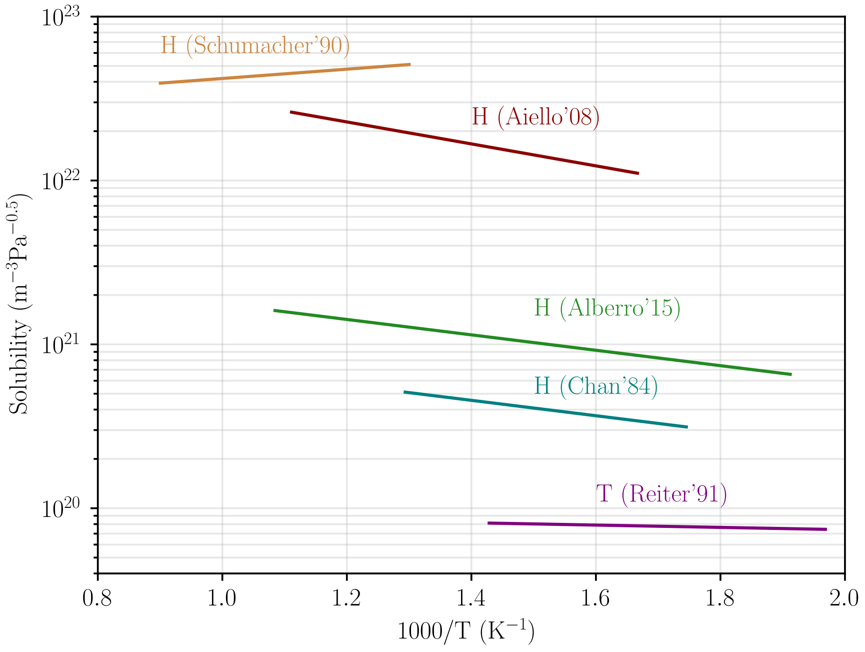
- Surface flux correlated to tritium source
- Lower flux in FW cooling channels

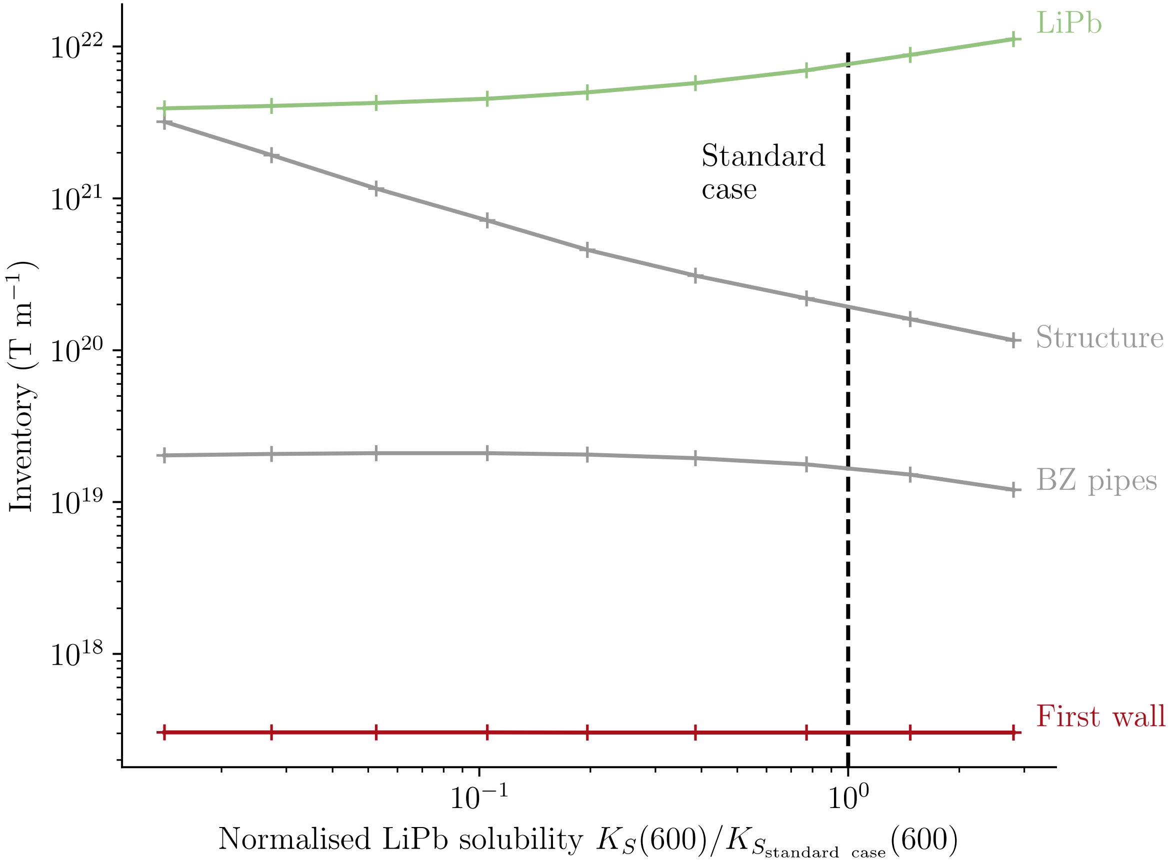
- Uncertainty in literature – Solubility of H in LiPb



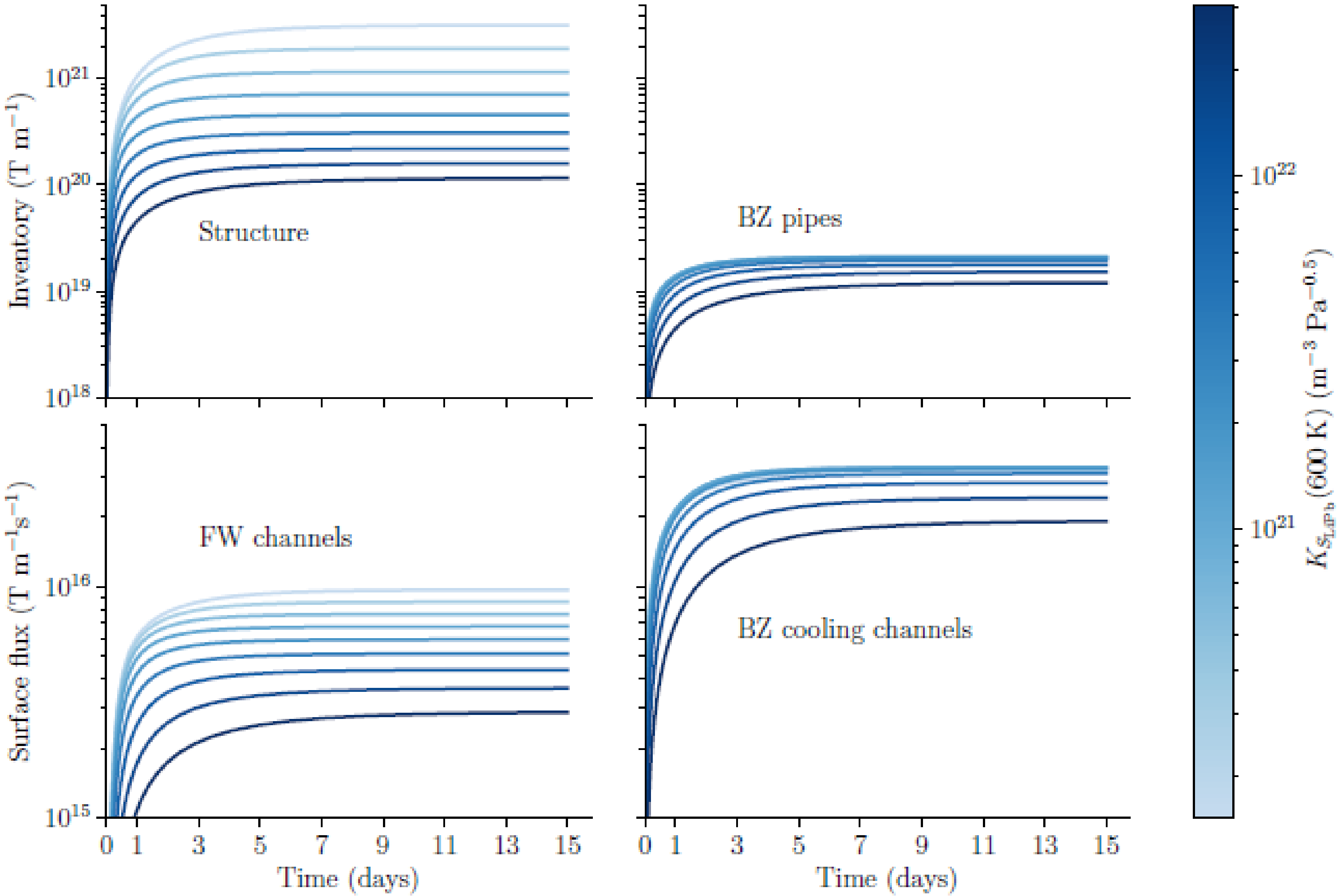


- Uncertainty in literature – Solubility of H in LiPb





- Uncertainty in the literature results in range:
  - Factor 25 difference in EUROFER inventory
  - Factor 3 difference in FW cooling channel surface flux


Structure
BZ pipes
FW channels
BZ cooling channels
Inventory (T m⁻¹)
Surface flux (T m⁻¹s⁻¹)
Time (days)
Time (days)
$K_{S_{\text{LiPb}}}(600\text{ K})\ (\text{m}^{-3}\ \text{Pa}^{-0.5})$

$$\text{heat flux} = h\,(T - T_c)$$

$$h = \text{Nu} \cdot k / d_w$$

Nusselt no.

$$\text{Nu} = f(\text{Re}, \text{Pr})$$

Reynolds no.

$$\text{Re} = \frac{\rho(P, T) \cdot \vec{u} \cdot L}{\mu(P, T)}$$

Prandtl no.

$$\text{Pr} = \frac{c_p(P, T) \cdot \mu(P, T)}{k\,(P, T)}$$

Velocity

$$\vec{u} = \frac{\dot{m}}{\rho(P, T) \cdot A}$$

f = Gnielinski correlation

k = thermal conductivity

d_w = wetted perimeter

ρ = density

L = characteristic length

μ = viscosity

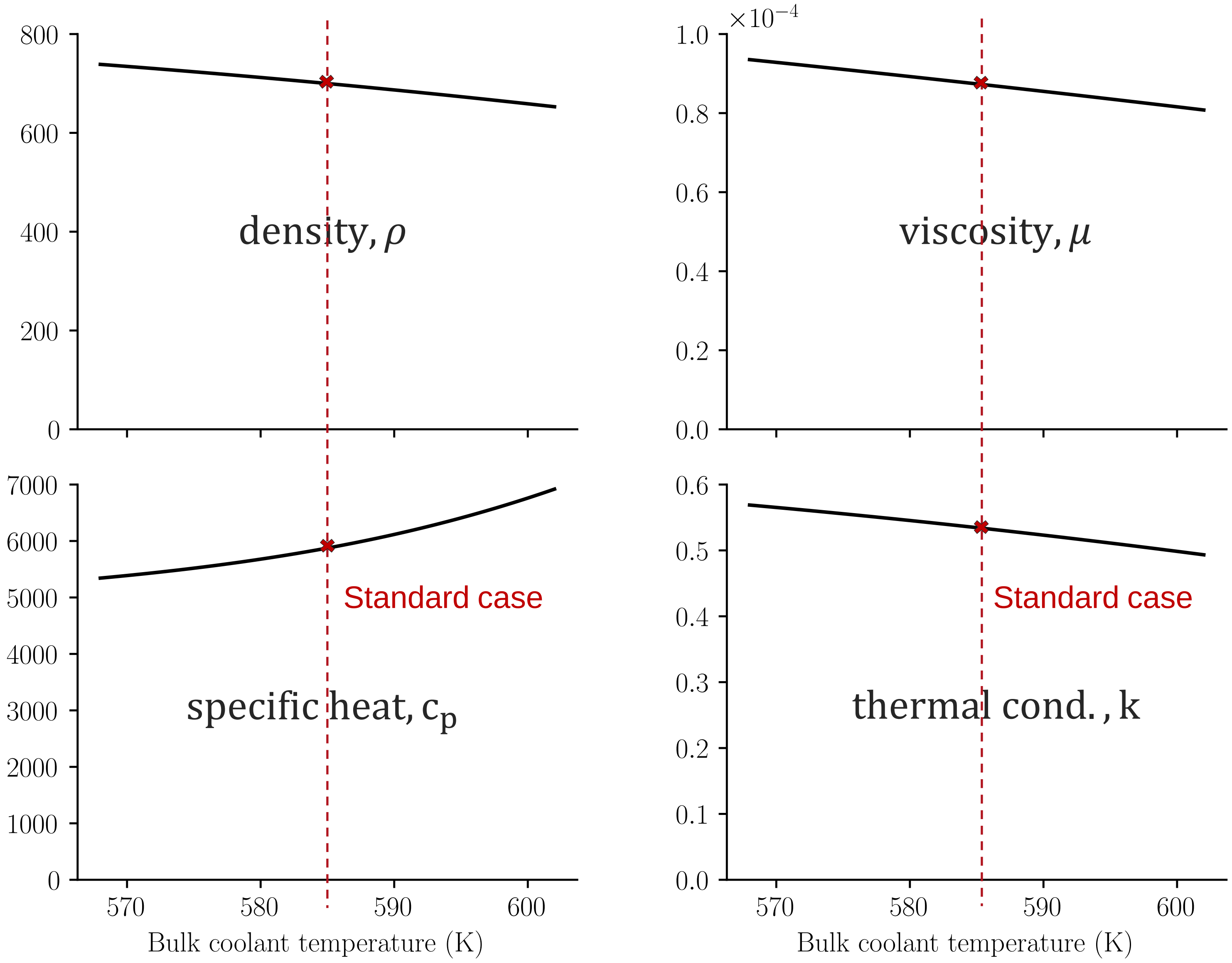
$\dot{m}$ = mass flow rate

A = Area

Expressions for water at 155 bar [1]:

Shown over temperature range of 569 - 601 K

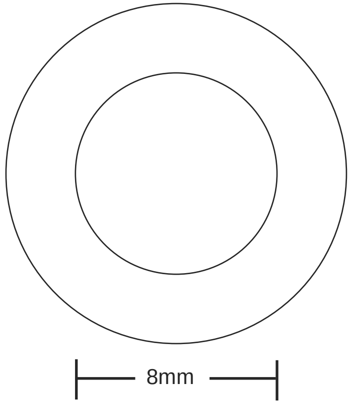
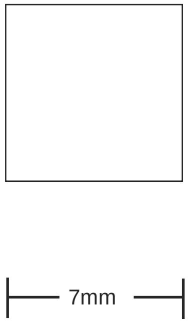
Standard case values at 585 K



$$h = \mathrm{Nu} \cdot k/d_w$$

$$\vec{u} = \frac{\dot{m}}{\rho(p,T) \cdot A}$$

$$\mathrm{Nu} = f(\mathrm{Re}, \mathrm{Pr})$$

	BZ pipes	FW Channels	units
			
	$d_{w,BZ} = 0.008 \cdot \pi$	$d_{w,FW} = 0.028$	$[\mathrm{m}]$
	$u_{BZ} = 1.73$	$u_{FW} = 4.60$	$[\mathrm{m\ s^{-1}}]$
	$\mathrm{Nu} = 235.8$	$\mathrm{Nu} = 464.2$	
	$h_{BZ} = 5.03 \times 10^3$	$h_{FW} = 8.87 \times 10^3$	$[\mathrm{W\ m^{-2} K^{-1}}]$

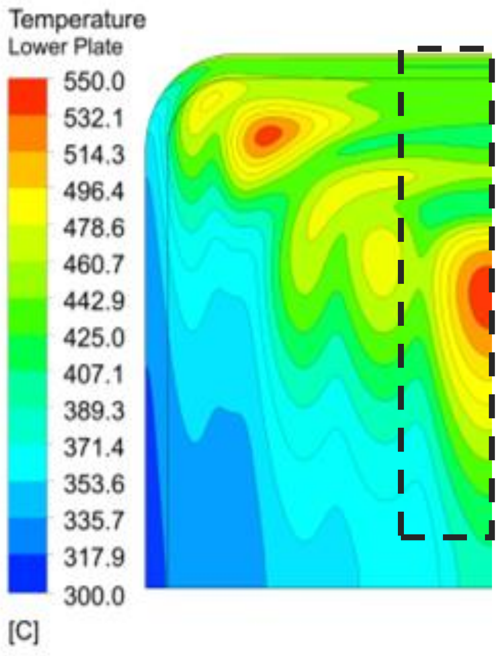
Results were compared against the literature [1]

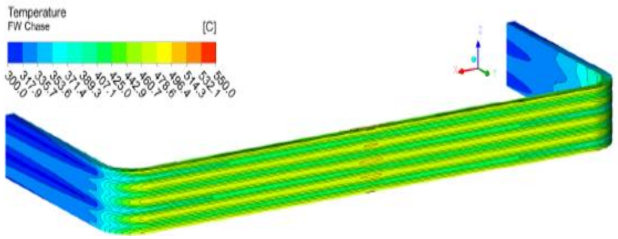
Results in good agreement with the designers reference

Suggesting that using a heat transfer coefficient works well

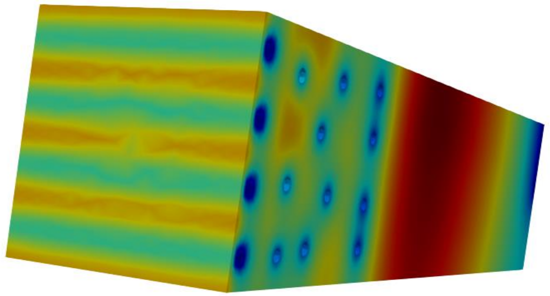
Is a reasonable replacement for modelling the water coolant

Reference [1]





My Results



Influence of heat transfer coefficient (h)

How does the heat transfer coefficient (h) influence flux of hydrogen into cooling channels?

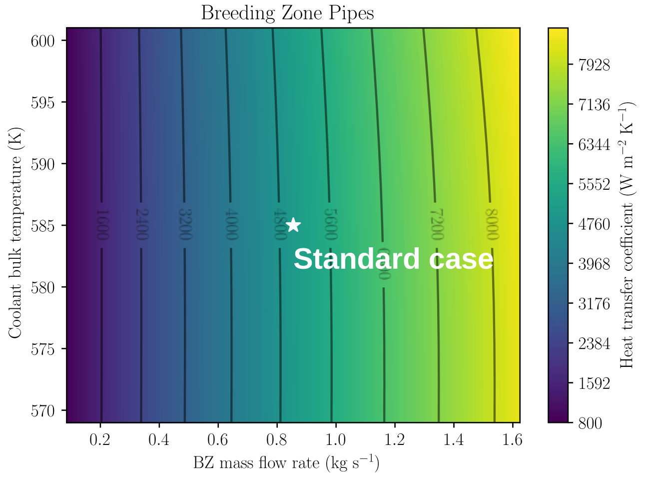
$$-\lambda \nabla T \cdot \mathbf{n} = h(T - T_c)$$

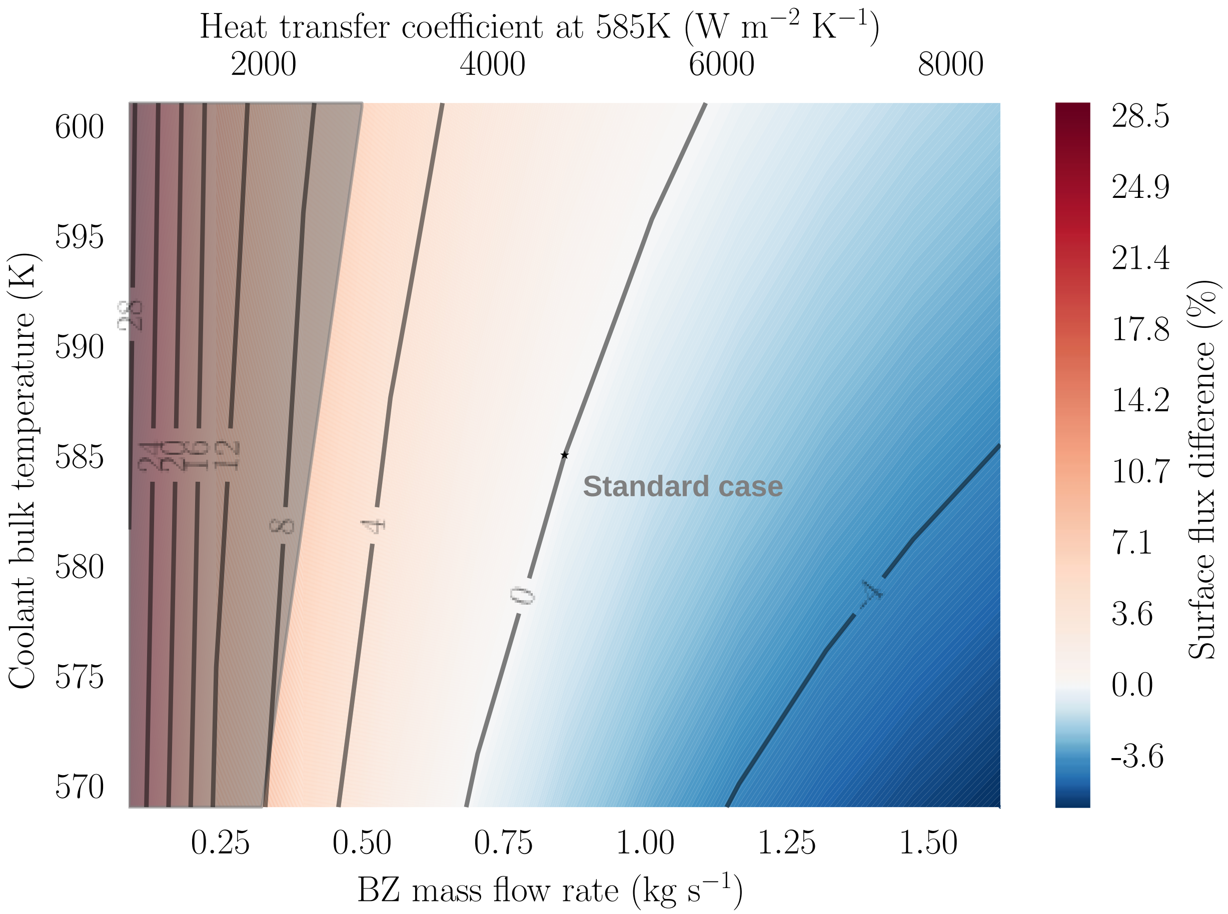
$$h = f(T, \dot{m})$$

Test range of T and $\dot{m}$:

$$569 < T < 601$$

$$0.1 < \dot{m} < 1.9$$





- Max **temperature** variation of **17 %**
- Max **surface flux** variation of **14 %**

In the case of just annealing:

$$\frac{\partial n_t}{dt} \quad \frac{\partial n_t}{dt} = \phi \cdot K \left[1 - \frac{n_t}{n_{\max,\phi}} \right] - A \cdot n_t \quad A \cdot n_t$$

$$n(t) = n_0 \cdot \exp(-A \cdot t)$$

Where:

$$A = A_0 \cdot \exp\left(\frac{-E_A}{k_B T} \right)$$

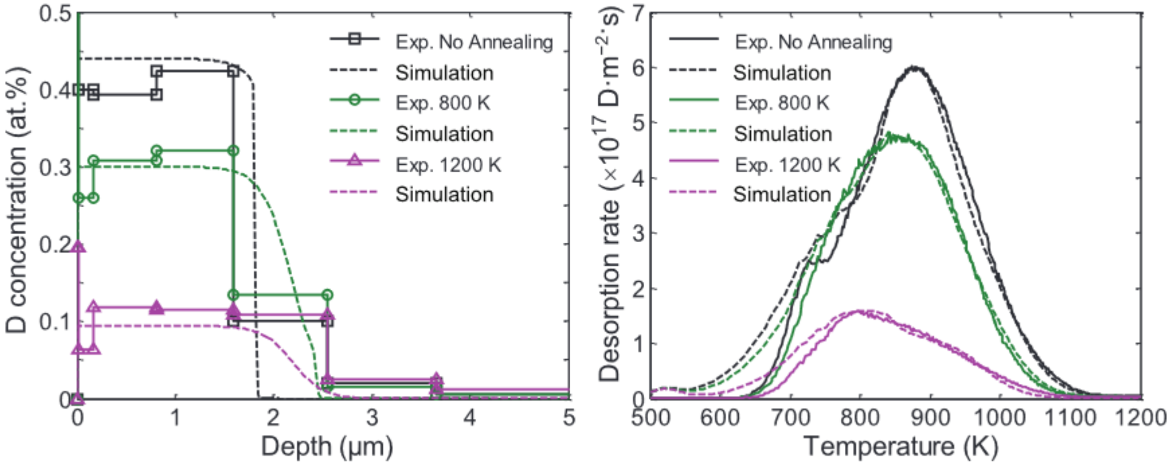
Self-damaged tungsten data [1]

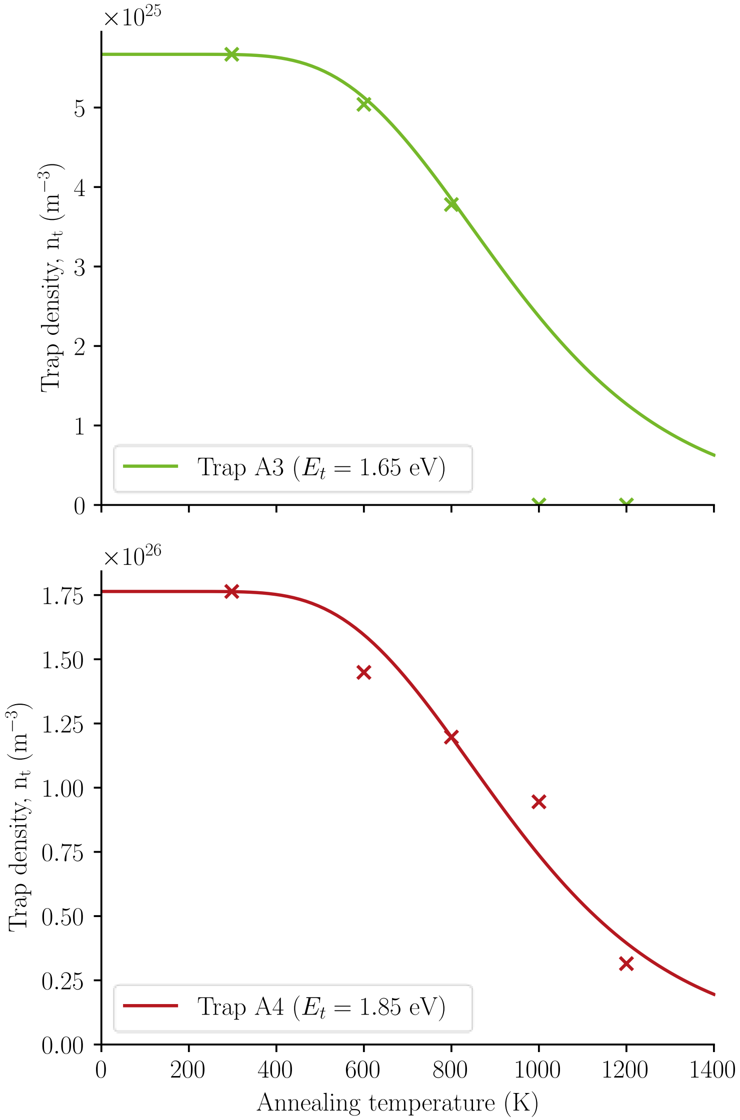
20 MeV W^{6+} ions at room temperature

Peak damage 0.5 dpa

Annealed in vacuum for 1h

TDS fitted – 3 damage induced traps





Hartmann number

$$Ha = B \cdot L \cdot \sqrt{\frac{\sigma_e}{\mu}}$$