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Tritium Transport Modelling: Current Status, Open Points and Perspectives

Italo Ricapito, F4E-TBM Programme

with contributions of: Luigi Candido and Carlos Moreno

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***Disclaimer**: this presentation deals with TTM for Breeding Blanket applications*

Legenda

HI Hydrogen isotopes
LMBL Liquid Metal Boundary Layer
TBS Test Blanket System
TTM Tritium Transport Modelling

Snapshot on the TTM development status

More and more interest is around Tritium Transport Modelling, especially for the breeding blanket development

Three are the main areas of application

- Calculation of the achievable TBR
- Analysis of the radiological hazard in the context of Safety Studies
- Design of tritium processing systems

Due to its natural domain TTM must deal with

- large systems composed by interconnected sub-systems (e.g. TBS in ITER)
- complex/multi-compartment components, with different materials (e.g. the BB module of He Cooled CB)

Snapshot on the TTM development status

Along the evolution towards the detailed design of different fusion machines, it is requested to have prediction capability of higher “fidelity” (reliability + accuracy)

The main challenges come from TTM inherent aspects

- Complexity in modeling the tritium transport in the bulk materials and interfaces
- Need to include elements of multi-physics to correctly describe the phenomenology of the tritium transport
- High sensitivity of the main outputs -typically tritium inventory and permeation rate- on several transport parameters
- Need for a stable and shared material parameters database, not easy to achieve

Snapshot on the TTM development status

Example: Complexity in modeling the tritium transport in the bulk materials and interfaces

Bulk materials

$$\frac{\partial C_s}{\partial t}+\sum_k \frac{\partial C^k_{s,t}}{\partial t} = -\nabla\cdot J_s + S_s - \lambda_s C_s - \lambda_s \sum_k C^k_{s,t} + \sum_m \lambda^s_m \left(C^s_m + \sum_k C^{s,k}_{m,t}\right)$$

transport equation in the bulk material

$$\nabla\cdot \mathbf{J}_s = \frac{d}{dx}\left[-D\left(\frac{dC_s}{dx} + C_s \frac{Q^*}{kT^2}\frac{dT}{dx}\right)\right]$$

diffusive flux of species “s”

Soret contribution

$$\frac{\partial C^k_{s,t}}{\partial t} = \alpha^t_{s,k}\frac{C^e_{t,k}}{N}C_s - (\alpha^r_{s,k}+\lambda_s)C^k_{s,t}$$

mass balance in the k_{th} trap type

where

C_s = solubilised concentration of species “s” atoms in the structure

J_s= diffusive flux of species “s” atoms

S_s = local source rate of species “s” atoms

$C^k_{s,t}$= concentration of atoms of species “s” in the “k_{th}” trap type

C^s_m= concentration of atoms of species “m” that decay into species “s”

$C^{s,k}_{m,t}$= concentration of atoms of species “m” that decay into species “s”

λ_s= decay constant of species “s” atoms

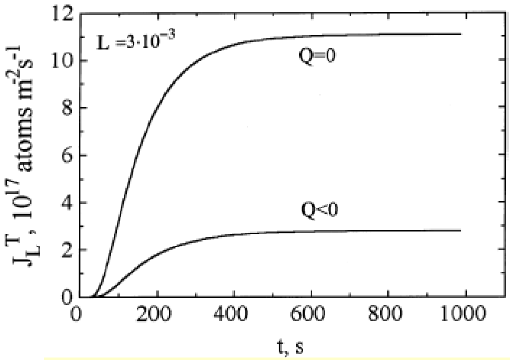
λ^s_m= decay constant of species “m” atoms that decay to species “s”

C^e_{tk}= concentration of empty traps of the “kth” type

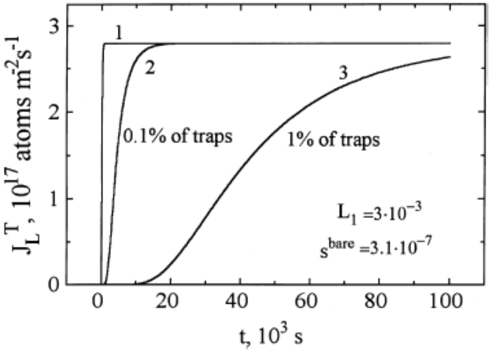
N= total trap concentration

$\alpha^t_{s,k}$= trapping rate coefficient of species “s” atoms in the trap type “k”

$\alpha^r_{s,k}$ = release rate coefficient for species “s” trapped atoms from



Effect of the Soret effect on the tritium permeation through the FW due to T impinging from plasma



Effect of the trap concentration: trap energy=0.63 eV

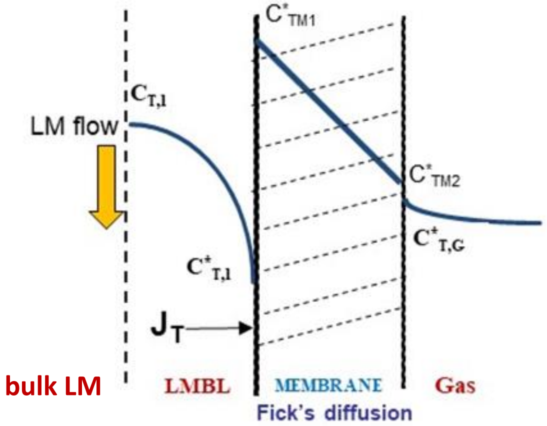
O. Ogorodnikova, JNM, 1999

Snapshot on the TTM development status

Example: Complexity in modeling the tritium transport in the bulk materials and interfaces

interfaces

LM-steel-gas



$$J_{T,LM} = h_{LM}\left(C_{T,L} - C^*_{T.l}\right)$$

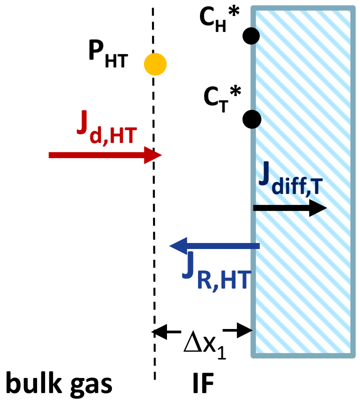
$$J_{T,diff} = D\left(\frac{\partial c}{\partial x}\right);\ c(O,L) = c^*_{TM1},\ c^*_{T,G}$$

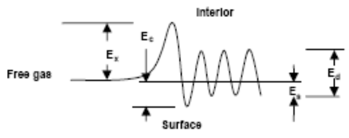
$$J_{T,G} = K_r c^{*2}_{T,G}$$

$$\frac{C^*_{T,M}}{C_{T,L}} = \frac{K_{S,M}}{K_{S,LM}}$$

The permeation number $W = \frac{\sigma K_1 p_h}{(\Phi/d)\sqrt{p_h}} = \frac{\sigma K_1 d}{\Phi}\sqrt{p_h}$

gas-steel-gas





$$J_{diff} = J_d - J_R$$

$$J_{d,HT} = K_{d,HT} \cdot \frac{\alpha P_T}{\sqrt{2\pi MkT}} \exp\left(-\frac{E_x}{kT}\right)$$

$$J_{R,HT} = K_r \cdot C^*_T \cdot C^*_H$$

$$\boxed{-D\frac{dC_T}{dx}\Big|_{x=0} = D\frac{(C_{1T} - C^*_T)}{\Delta x_1} = K_d \cdot P_T - K_r \cdot C^*_H C^*_T}$$

Give the importance of the diffusive transport over the surface phenomena

Snapshot on the TTM development status

Several models available for the Breeding Blanket Community in form of customized numerical and analytical codes.

Component-Level Codes, e.g.
- TMAP7
- TESSIM-X
- TTM in COMSOL Multi-physics

System-Level Codes, e.g.
- EcosimPro
- Theta FR
- FUS-TPC
- ModAn

Because of the increasing computational capacity, each of the two families goes in the direction to take features of the other

- Extension of the analysis domain for the component-level models
- Introduction of more physical elements in the system-level models

In general, the tendency of the physicist and developers is to increase "fidelity" of the prediction capability. This requires an effort in two areas:

- implementation into the main transport model of relevant elements of multi-physics / accuracy
- use of a well established physical property material database / reliability

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Implementation of Multi-physics Approach

General

The most relevant elements of multi-physics to be incorporated in the main TTM to increase the model fidelity

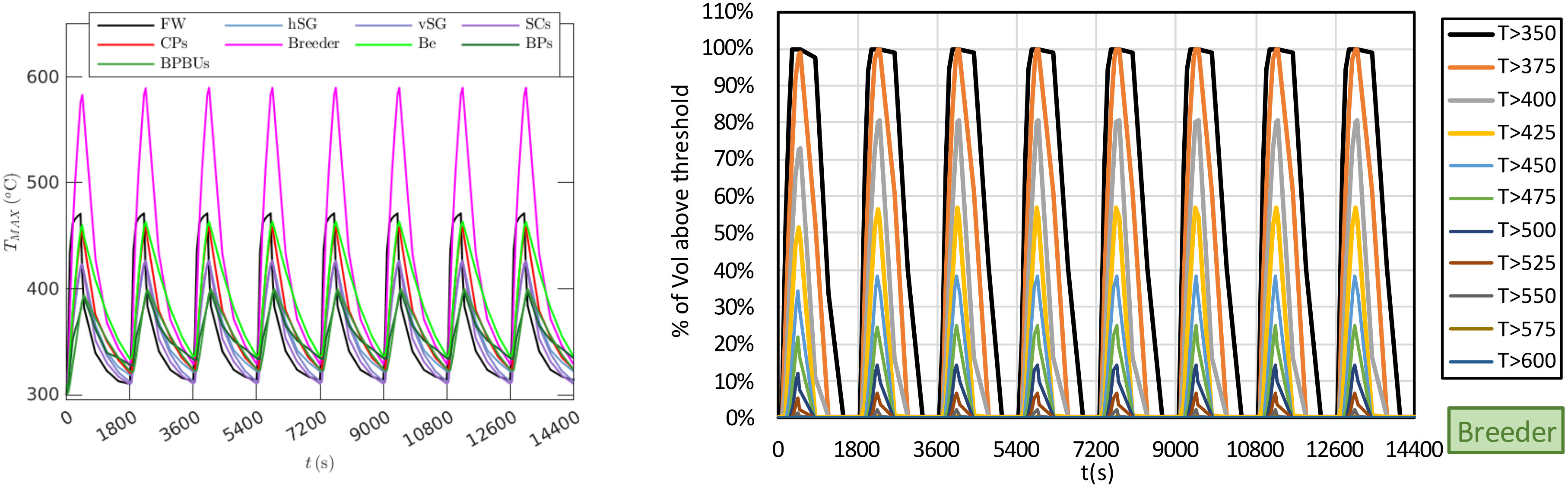
- the temperature field coupled with neutronic analysis, either at steady state (power reactor) and in transient conditions (Test Blanket System)
- the chemistry of the purge/coolant and co/counter permeation
- tritium trapping under irradiation
- MHD effects for the relevant breeding blanket concepts and TBS
- **for system-level models**, the integration of specific functional models. This could be focused on components playing a relevant function in the tritium migration path, like tritium extractors from Pb-16Li, adsorption/getter beds for HI concentration in gas mixtures

Implementation of Multi-physics Approach

Temperature Field/Neutronics - 1

Coupling the tritium transport equations with the temperature field, even variable with the time, of a component or system generating or containing tritium is of primary importance to increase the accuracy of the model.

This is particularly evident for the highly heterogeneous BB concepts, like the ones based on CB-Be-He



HCCP-TBM: preliminary analysis of the CB thermal field for the ceramic breeder *(E. Rodriguez, F. Rueda, Esteyco, 2023)*

- nuclear heat: 300 kW;
- surface heat flux: 0.25 MW/m^2
- n. 8 back to back pulse series with: FT= 300 s; repetition time= 1800 s
- Volumetric heat deposited as per MCNP analysis

Implementation of Multi-physics Approach

Temperature Field/Neutronics -2: *Tritium Inventory in Li_4SIO_4*

Lumped model of "tritium residence time" τ for the tritium inventory in the OSI bed

$$I(t) = I(0) + G \cdot \tau \cdot \left[1 - \exp\left(-\frac{t}{\tau}\right)\right]$$

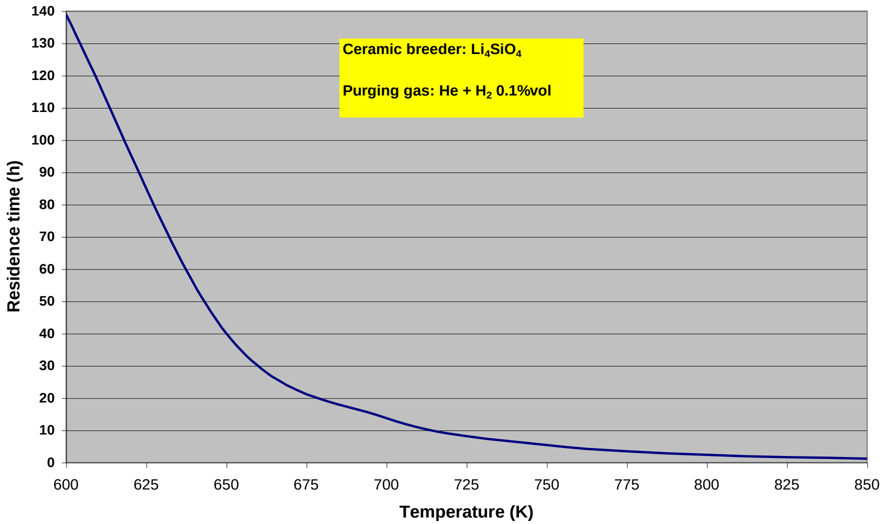
$$I_{ss} = I(0) + G \cdot \tau$$

$$\tau = \frac{1}{K_d}$$

K_d: the overall tritium transfer coefficient

I_{SS}: the tritium inventory at the steady state

G: the tritium generation rate inside the OSI bed



He+0.1%vol of H_2 purge gas (Van der Laan et al.,

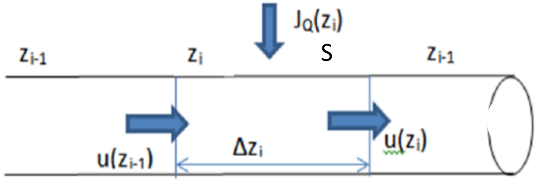
Results for the tritium inventory for a steady state BB with a tritium generation rate of 100 g/day

Lumped model with the average temperature and flat TGR profile	Lumped model with the average temperature and exp. TGR profile	Lumped model with 1D temperature repartition and exp. TGR profile
I_{avT}= 77.8 g	**I_{avT}= 29.27 g**	**$I_{1D\text{-}T}$= 23. 9 g**

For system-level codes it is of outstanding importance the use of a realistic TGR profile and 1D radial temperature discretization

Implementation of Multi-physics Approach

Chemistry and co/counter HI transport



HI mass balance in the purge gas of HCCP-TBM

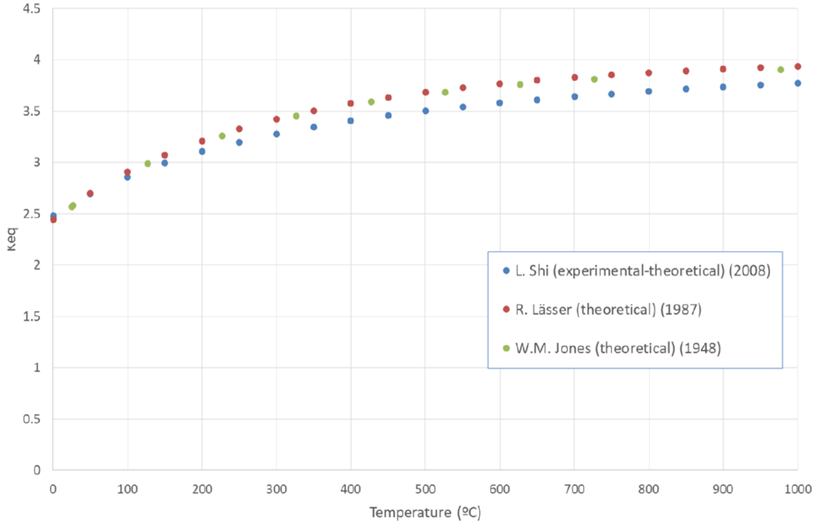
$$\frac{dc_{Q2}(t,z_i)}{dt} = -\frac{u(z_i)}{\Delta z}c_{Q2}(t,z_i) + \frac{u(z_{i-1})}{\Delta z}c_{Q2}(t,z_{i-1}) + \overbrace{J_{Q2}(t,z_i)}^{Q_2\text{ ingress from an external source}}\cdot S + \underbrace{\chi_{Q2}(t,z_i)}_{Q_2\text{ generation rate}}$$

C= mass of Q_2

H_2 + HTO ↔ HT + H_2O [1]

H_2 + T_2 ↔ 2HT [2]

$$\chi_{HT}(t,z_i) = -k_1 c_{HT} c_{H2O} + k_2 c_{HTO} c_{H2} + 2k_3 c_{T2} c_{H2} - k_4 c_{HT}^2$$



Equilibrium constant vs temperature for the reaction H_2+HTO ↔ HT + H_2O

HI concentration [mol m^{-3}] at the outlet of the He purge gas for HCCP-TBM; He pressure 4.5 bar, H_2 inlet 0.1%$_{vol}$

T(°C)	300	500	700	900
C_{H2}	4.56E-02	4.56E-02	4.56E-02	4.56E-02
C_{H2O}	4.56E-02	4.56E-02	4.56E-02	4.56E-02
C_{HT}	1.13E-05	1.03E-05	9.78E-06	9.46E-06
C_{HTO}	5.19E-06	6.17E-06	6.71E-06	7.04E-06
C_{T2}	8.18E-10	6.34E-10	5.48E-10	5.01E-10

Study by C. Moreno et al., Ciemat, 2018

- HTO becomes more and more relevant as the temperature increases, due to the shape of the eq. constant vs. temperature of reaction [1]
- the large excess of H_2 in the purge gas leads to the negligible production of T_2, as per the reaction [2]

Implementation of Multi-physics

Chemistry and co/counter HI transport

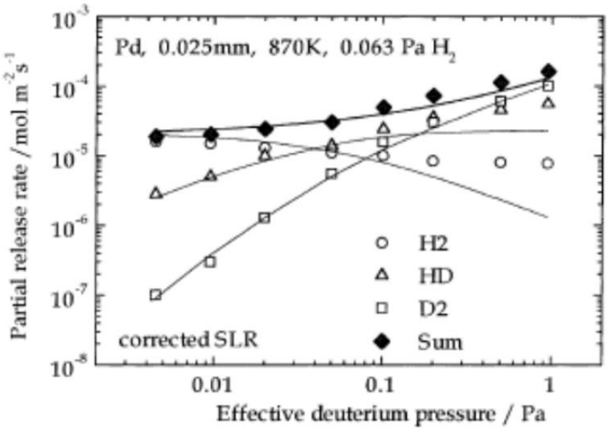
BULK DIFFUSION

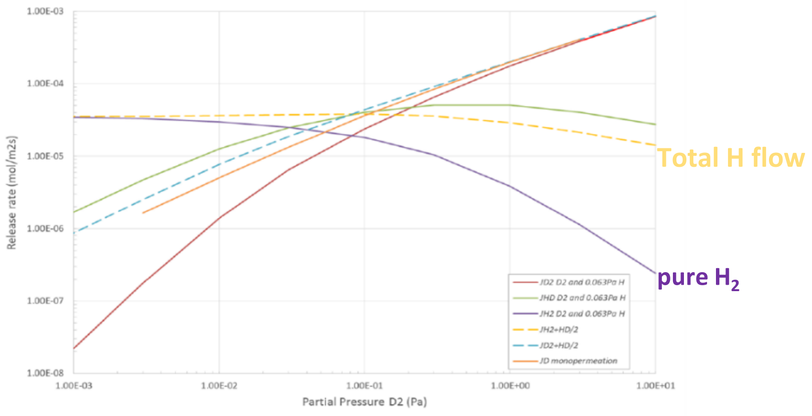
$$J = \underbrace{-D\left(\frac{\partial C}{\partial x}\right)\left(\frac{N - C_Q}{N}\right)}_{\text{Classic term}} \underbrace{- D\,\frac{C}{N}\left(\frac{\partial C_Q}{\partial x}\right)}_{\text{Isotopic term}}$$

- In most of the cases, the lattice density is high enough for the factor $(N - C_Q)/N$) to be 1
- In the particular case of HCPB-TBS conditions, where the molecular density of EUROFER is 1.38x10^5 mol/m^3 and the concentration of hydrogen and tritium are 0.7 mol/m^3 and 1.65x10^{-5} mol/m^3 respectively, no isotopic effects take place in the bulk

SURFACE ISOTOPIC EXCHANGE

Experiment by Kizu: permeation with increasing D_2 partial pressure with a fixed H_2 partial pressure (0.063 Pa) on the pressure side





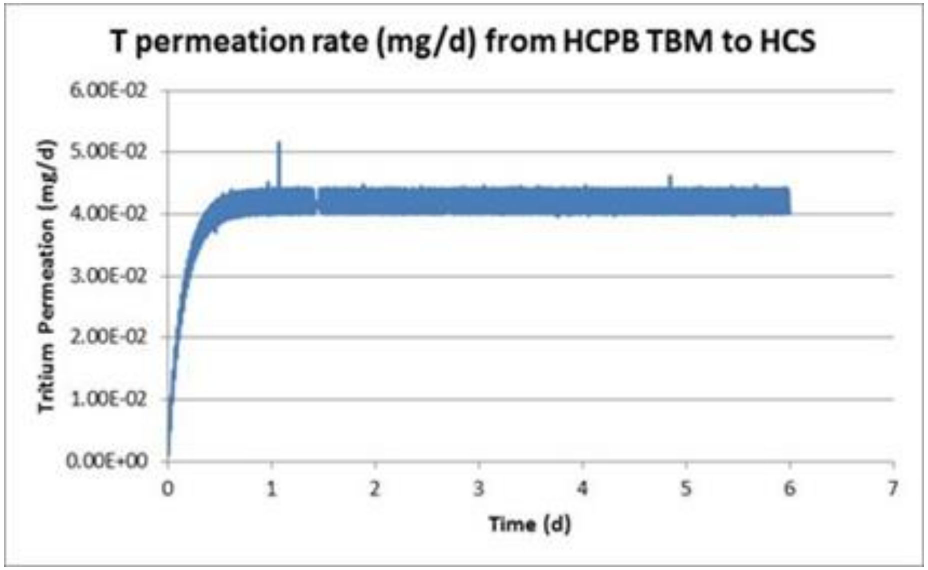
Fitting of Kizu's results with the EcosimPro code

H-D on the same side (*co-permeation*): the effect of increasing H_2 partial pressure is to reduce the tritium flux entering the solid metal because of the increased backward HT recombination flux

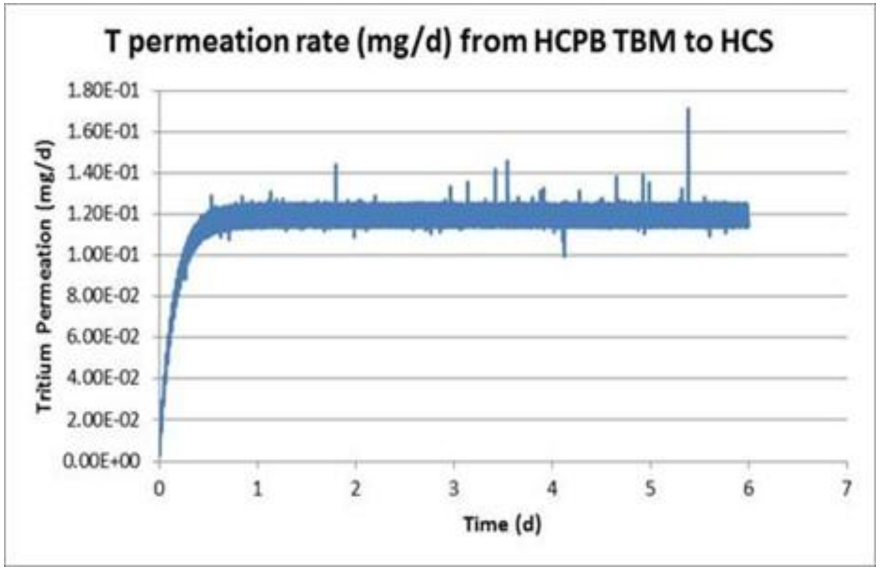
Implementation of Multi-physics Approach

Chemistry and co/counter HI transport

effects of H/T co-diffusion from He purge gas, simulation runs by EcosimPro



Tritium permeation rate from HCPB-TBM to HCPB-HCS, **400 Pa of H_2** in He purge stream, 6 days of back to back inductive pulses



Tritium permeation rate from HCPB-TBM to HCPB-HCS, **40 Pa of H_2** in He purge stream, 6 days of back to back inductive pulses

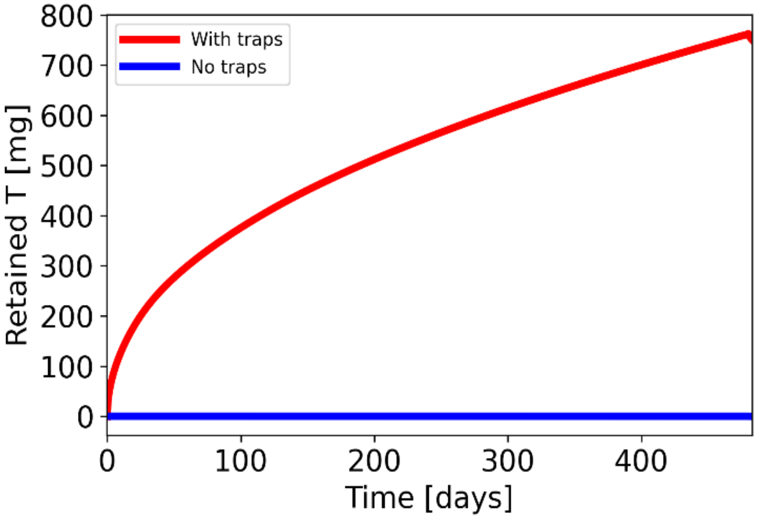
Implementation of Multiphysics

Tritium trapping

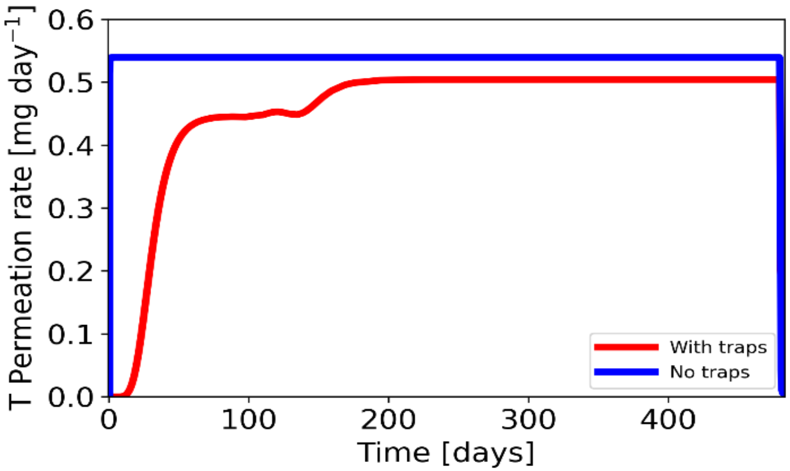
Two main effects, extremely significant

- increase of the tritium inventory
- Delay of the tritium permeation (e.g. into the main coolant)

Tessim-X prediction on WCLL-TBM in ITER



Tritium inventory in WCLL-TBM box with and without traps (0.17 mg) during a full irradiation campaign in ITER



Evolution over the time of the tritium permeation rate into the water coolant with and without traps during a full irradiation campaign in ITER

Arredondo, Schmidt, 2022, KIT, 2022

the low HI solubility of the RAFM steels (e.g. EUROFER) used for BB and TBS is the reason why the tritium retention is driven by the trapping in the lattice defects more than by its solubilization

Implementation of Multiphysics

Tritium trapping

Incorporation of the tritium trapping phenomena in TTM

Important for a steady state machine:

- for the tritium inventory assessment in nominal conditions
- for hazard quantification (e.g. in-vessel LOCA)

Essential for pulsed Machines (TBS in ITER, pulsed DEMO, etc.)

- for the dynamic tritium inventory calculation: flat top, ramp-down + dwell
- for hazard quantification (e.g. in-vessel LOCA)

Implementation of Multiphysics

MHD effects

Study case: radial pipe in EUROFER, located in the pipe forest connecting the HCLL-TBM with the Port Cell.

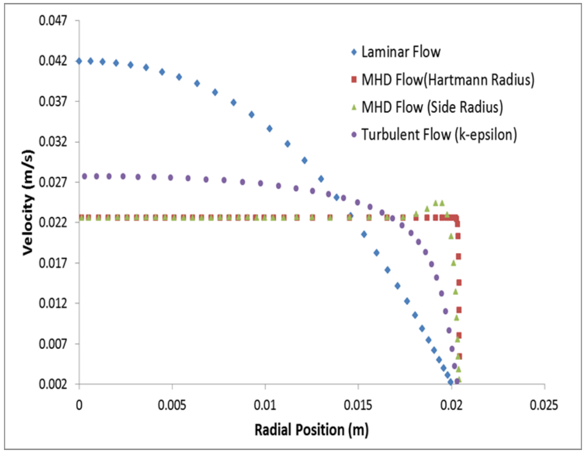
Model developed in Ansys Fluent (C. Moreno et al., 2018)

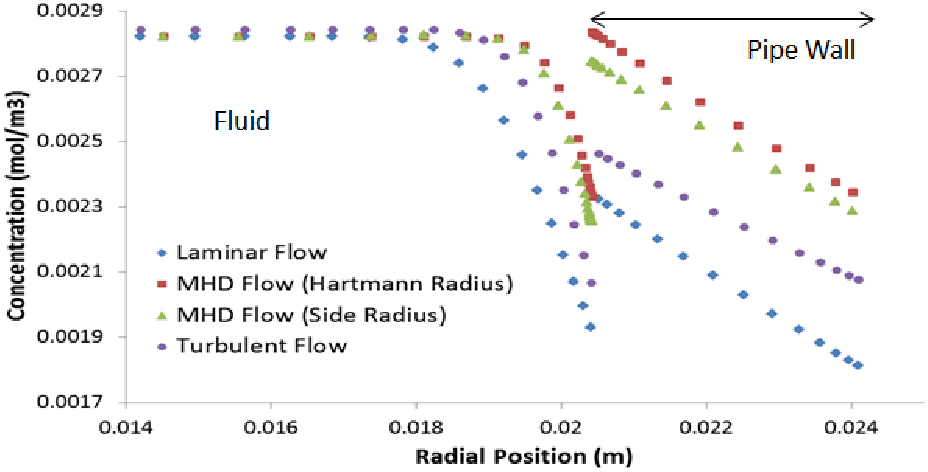
T (K)	623
K_s PbLi (mol/m^3 Pa$^{0.5}$)	1.00e-3
K_s Wall (mol/m^3 Pa$^{0.5}$)	1.22e-3
D PbLi (m^2/s)	9.34E-10
D Wall (m^2/s)	3.56e-09

K_r Wall (m^4/s mol)	7.14e-05
K_d Wall (mol/m^2 s Pa)	1.06E-10
c inlet (mol/m^3)	2.82e-03
P_{ext} (Pa)	0

U_0 (m/s)	0.0225
D_{ext} (m)	0.0483
th_{Wall} (m)	0.00368
L (m)	7.769

B_0 toroidal (T)	1.5
B_0 poloidal (T)	0.75
Ha	719





The velocity and the concentration boundary layers are shrunk by the magnetic field, with the consequent higher tritium permeation due to the higher tritium concentration at the metal surface

	Laminar case	Turbulent Case	MHD Case
Permeation (g/day)	1.55E-04	1.96E-04	2.50E-04
Inventory Steel (g)	2.55E-05	2.78E-05	8.61E-05
Inventory PbLi (g)	8.47E-05	8.63E-05	3.14E-05

Implementation of Multiphysics

MHD effects

The value of average mass transfer coefficient (K_T) and the thickness of the boundary layer can be obtained from the ANSYS-Fluent models

	Kt (m/s)	Sh	δmid (mm)
Laminar	7.00E-07	30.68	1.8
Turbulent	9.97E-07	43.70	1.3
MHD fully developed	2.04E-06	89.49	0.8

Beneficial to directly impose in the main TTM the mass transfer boundary conditions in the interface PbLi/steel taken by a specific analysis and use it in the tritium transfer equation across the LMBL

$$J_T = K_T \cdot (c_{bulk} - c_{int})$$

Implementation of Multiphysics

Incorporation of simplified functional models

In most of the current system-level models, **performance parameters** of components implementing a relevant function (e.g. tritium extractor from Pb16Li, tritium extraction from He purge gas, heat exchanger, etc.) **are imposed as input data**.

The direct incorporation of simplified functional models of the above components increases the global accuracy without significantly impacting the computational load

Example

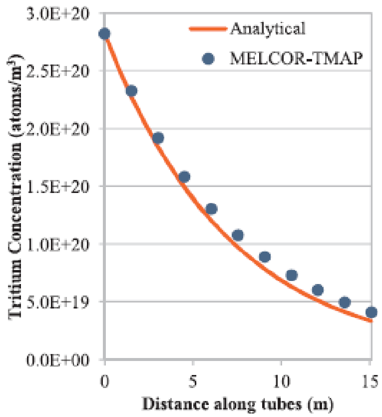
Instead of imposing a tritium extraction efficiency for PAV in the PbLi loop of a PbLi based BB (WCLL, HCLL, DCLL), it could be used a simplified analytical model which gives the tritium concentration in PbLi bulk in the advection direction

$$C_B(z) = C_0 \exp\left(-\frac{4K_T z}{vd}\frac{\zeta}{1+\zeta}\right)$$

$$\zeta = \frac{2\Phi}{K_T K_S d \ln(d_o/d)}$$

ϕ= permeability in the solid
K_T= mass transfer coefficient in LM
K_S= Sievert's constant in the LM

B. Merril., P. Humrickhouse et al., Fus. Eng&Des., 2010



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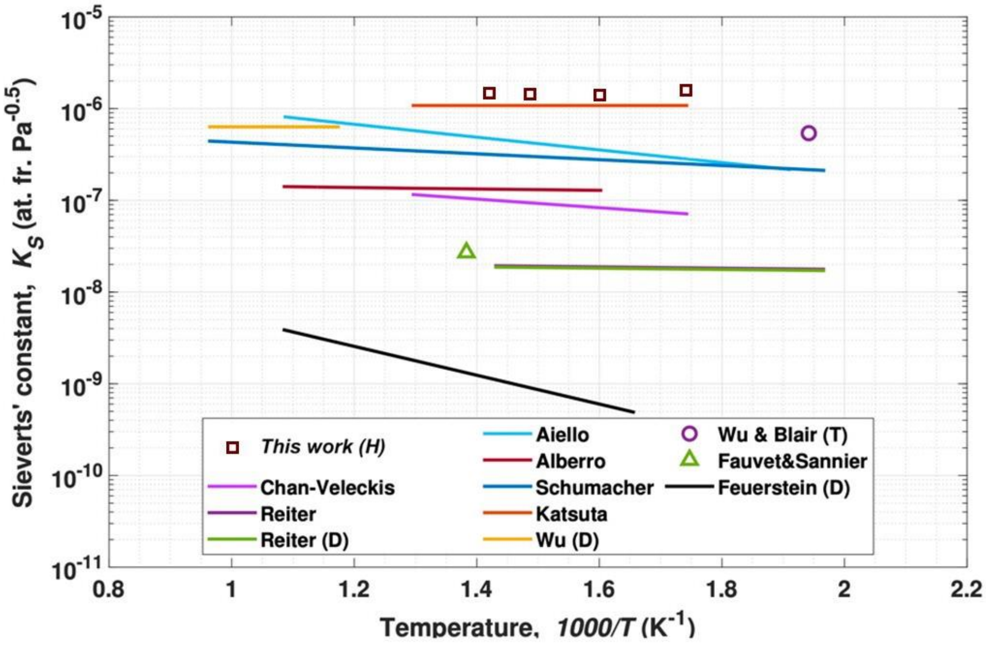
Materials Property Database

The impact of the materials properties on the reliability of the TTM prediction capability is, in general, extremely high: this comes directly from the physics of the tritium transport

It is then of outstanding importance to select the most reliable values and correlations for the many physico-chemical parameters used in the models and connected multi-physics subroutines

A first tentative data selection is given here

- changes have to be evaluated
- new data are under production
  - New values of K_r and Kd on EUROFER (CIEMAT)
  - New values of K_s for PbLi



Ciro Alberghi et al. , this Conference

Materials Property Database

PARAMETER	CORRELATION	MEAS. UNIT	Notes
Sieverts' constant Pb-16Li/T	0.237·exp (-12844/RT)	mol m^{-3} $Pa^{-1/2}$	Aiello, Fus. Eng&Des., 2006 Waiting new data on Hyper-Quarch II
Diffusivity Pb-16Li/T	4.03·10^{-8}·exp(-19500/RT)	$m^2 \cdot s^{-1}$	Reiter, 1991
Sieverts' constant Eurofer/T	2.25·10^{-2}·exp(-15100/RT)	$mol \cdot m^{-3} \cdot Pa^{-0.5}$	Esteban et al., JNM 2007
Diffusivity Eurofer/T	4.57·10^{-7}·exp(-22300/RT)	$m^2 \cdot s^{-1}$	Esteban et al., JNM 2007
Recombination coefficient Eurofer/T	2.84·10^{-7}·exp(-28679/RT)	$mol^{-1} \cdot m^4 \cdot s^{-1}$	Data for Optifer: under production new data for EUROFER97
Sieverts' constant AISI-316L/T	1.47·exp(-20600/RT)	$mol \cdot m^{-3} \cdot Pa^{-0.5}$	Forcey, 1988
Diffusivity AISI-316L/T	7.66·10^{-8}·exp(-42500/RT)	$m^2 \cdot s^{-1}$	Forcey, 1988
Recombination coefficient AISI-316L/T	6.03·10^{-5}·exp(-16721/RT)	$mol^{-1} \cdot m^4 \cdot s^{-1}$	Forcey, 1988
T transfer coefficient through LMBL	$\frac{h_m \cdot D_{tube}}{D_{PbLi}} = 0.0096\ Re^{0.913}\ Sc^{0.346}$	m/s	Selection proposed by S. Willms (2007)
T residence time for Li_4SiO_4 (for He purge with H_2= 0.1$\%_{vol}$)	τ (T) = 2.28·10^5 · exp (-9270/T)	h	Exotic-8 campaign
T residence time in for Li_2TiO_3 (for He purge with H_2= 0.1$\%_{vol}$)	τ (T)= 1.995 10^{-6} exp (10315/T)	h	Exotic-8 campaign

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Summary&Recommendations

1. The large interest on TTM has led to a proliferation of codes and tools at component and system level, triggered by the more and more available high computational capacity. However, there was a lack of coordinated effort among the different actors

2. Implementation of multi-physic elements is extremely important, not only for component-level but also for the system-level models. This is possible now thanks to the availability of a much higher computational capacity

3. For the system-level codes, it is of primary importance to incorporate
    - the temperature field in the BB/TBM modules because of its implication in terms of tritium inventory and permeation into the coolant
    - tritium trapping in the manufacturing and irradiation traps
    - the main chemical effects and the phenomena of co and counter-permeation
    - MHD effects when relevant
    - simplified, possibly analytical, component models (e.g. tritium extractor, heat exchanger) with explicit dependence on the thermo-hydraulic conditions

4. Adopting a common material database would be very beneficial in order to make meaningful the exchange of results among the different communities. This approach was done, under the umbrella of IO for the update of the PrSR, and the results were really positive.

Summary&Recommendations

4. Adopting a common material database would be very beneficial in order to make meaningful the exchange of results among the different communities. This approach was done, under the umbrella of IO for the update of the PrSR, and the results were really positive.

5. On the interface: try always go use a general transport regime whatever is the ***permeation number*** W. This because also the W number can vary as a function of space and time so that imposing a particular transport regime is always risky.

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