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Letter to the Editors

Calculations of the tritium re-emission rate in the DEMO first wall

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Abstract

The deuterium and tritium re-emission fluxes from the first wall (FW) of the DEMO reactor have been calculated. The influence of temperature of the first wall (FW), surface conditions, and trapping in neutron-produced defects on the tritium re-emission rate has been considered. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

In the case of controlled fusion by magnetic confinement, as it will occur in the demonstration reactor DEMO, hydrogen isotope recycling from the first wall (FW) influences the plasma exhaust during discharge. When the fast hydrogen isotopes interact with the metal, the fraction of the implanted particles is directed back from the surface with the reflection coefficient r and reenters the plasma, while the remaining fraction penetrates in the metal. The penetrated fraction diffuses in the metal. When a diffusing atom reaches the plasma-facing surface, it recombines with another atom at the surface to desorb as a hydrogen molecule. The hydrogen recycling is characterised by two components: (i) the fast one from backscattering and (ii) the other from surface recombination. Analytical models [1–3] and numerical codes [4–8] have been developed for the calculations of recycling, inventory and permeation of hydrogen isotopes in fusion reactor design concepts. The purpose of the present investigation is to calculate the deuterium and tritium re-emission rates from the FW of the DEMO reactor due to hydrogen isotope surface recombination.

2. Input data: diffusivity, solubility and sticking factor for hydrogen isotope/first wall interaction

It is assumed that the FW is represented by a thickness $L_1 = 3 \times 10^{-3}$ m of 7–10% Cr martensitic steel between plasma and FW coolant. The martensitic steel F82H belongs to the 7–10% Cr martensitic steel class that have undergone some modification in order to achieve better low-activation characteristics compared with those of MANET. The F82H steel is close to the material assumed to be used for the first wall and structure for the demonstration fusion reactor DEMO. The data of deuterium solubility $K_s^D = K_{s0}\exp(-Q_s/kT)$ and diffusivity $D_D = D_0\exp(-E_m/kT)$ in F82H steel are taken from [9] and are presented in Table 1. The tritium extrapolated value D_T for the diffusivity in the F82H steel is defined using the classical diffusion theory:

$$D_T = \sqrt{m_D/m_T}D_D = \sqrt{2/3}D_D. \tag{1}$$

The association desorption J_{0i} of the ith hydrogen isotope on the surface is usually described in terms of the 'recombination coefficient' K_r^i [10–16]:

$$J_{0i} = 2K_r^i u_{0i}^2, \tag{2}$$

where u_{0i} is the concentration of the ith hydrogen isotope near the plasma-facing side.

According to [14–16] K_r^i equals the relation of the adsorption coefficient to the square of Sieverts' constant:

$$K_r^i = (k_{ad})_i/K_s^2. \tag{3}$$

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Table 1
Materials data for the deuterium-F82H system

Property	
D_0 (m^2/s)	1.07×10^{-7}
E_m (eV)	0.144
K_{s0} (atoms/m^3 $\sqrt{\text{Pa}}$)	4.52×10^{23}
Q_s (eV)	0.278

The adsorption coefficient k_{ad} was obtained in Ref. [17] for the interaction of deuterium with bare martensitic steel MANET. It is more common to use the sticking coefficient $s = s_0 \exp(-2E_c/kT)$ ($k = 8.618 \times 10^{-5}$ eV/K) instead the adsorption coefficient:

$$(k_{ad})_i = s\mu_i \text{ (molec. m}^{-2}\text{ s}^{-1}\text{ Pa}^{-1}), \tag{4}$$

where μ_i is defined by the kinetic theory expression $\mu_i = 1/\sqrt{2\pi m_i k_B T}$ (m_i is the mass of the ith hydrogen molecule and $k_B = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant). Using Eqs. (3) and (4), the recombination coefficient is a function of the sticking coefficient:

$$K_r^i = s\mu_i/K_s^2 \text{(molec. atoms}^{-2}\text{ m}^4\text{ s}^{-1}). \tag{5}$$

The plasma-facing surface may be sputter-cleaned during plasma operation. The sticking coefficient for such an extremely clean surface is often close to unity ($s \cong 1$) [18,19]. This means that the adsorption coefficient for the ith hydrogen isotope for a perfectly cleaned surface is

$$(k_{ad})_i^{\text{clean}} = \mu_i \text{(molec. m}^{-2}\text{ s}^{-1}\text{ Pa}^{-1}). \tag{6}$$

The data of adsorption and sticking coefficients of a bare steel surface (presence of small amounts of impurities on the surface) for the deuterium-MANET interaction [17] as well as of a sputter-cleaned surface are presented in Table 2. The adsorption coefficient of the tritium–martensitic steel interaction such as MANET and F82H is defined by

$$(k_{ad})_T = (k_{ad})_D\sqrt{m_D/m_T} = (k_{ad})_D\sqrt{2/3}. \tag{7}$$

The incident tritium ion flux to the first wall of DEMO is $I_0 = 3 \times 10^{20}$ atoms m^{-2} s^{-1} (50% D and 50% T) extrapolated from ITER conditions [20]. The deposition of the penetrating ions (implantation depth) $R_p = 5 \times 10^{-9}$ m is also extrapolated from ITER conditions [20]. The temperature $T = 741$ K on the plasma-facing side of the FW is taken from Ref. [21].

3. Results and discussion

3.1. Surface effects

The calculations of the deuterium and tritium re-emission rates were performed using the model in Ref. [22]. The time dependence of the tritium re-emission flux J_0^T for different conditions on the plasma-facing surface is shown in Fig. 1. The re-emission flux reaches the steady state within a relatively short time of the order of $\tau \approx 1$ s. One of the factors which strongly influences the time τ to reach the steady state is the condition on the plasma-surface side, namely the sticking coefficient. The increase of the sticking probability strongly reduces the recycling time τ.

We can roughly estimate the re-emission rate by the following expression derived in Ref. [2] (Fig. 2):

$$J_0(t) = I_0(1 - \sqrt{R/I_0 t\pi}), \tag{8}$$

where $R = D_i/2K_r^i = D_i K_s^2/2\mu_i s$ (atoms m^{-2}) is the so-called recycling coefficient. With increasing s, the recycling coefficient R decreases as shown in Fig. 1. From Eq. (8) follows that the reduction of the recycling coefficient R (i.e. increase of s or decrease of impurities from the surface) decreases the recycling time.

It is noteworthy that there are two quasi-steady states (Fig. 1): (i) the first during a very short time is due to the release of implanted tritium from sub-surface layers and (ii) the second during longer time is due to tritium coming from deeper layers.

Since both diffusion and recombination coefficients are mass dependent, the recycling coefficient $R = D_i/2K_r^i$ does not depend on the mass of the hydrogen isotope and is the same for all hydrogen isotopes. From Eq. (8) follows that the re-emission flux $J_0(t)$ is mass independent but, as shown later by numerical calculations, it is not correct.

3.2. Isotopic effects

From Eq. (5) follows that the recombination coefficient is inversely proportional to the square root of the mass of the ith hydrogen isotope, $K_r^i \sim 1/\sqrt{m_i}$. Consequently, the deuterium release rate is slightly faster than that of tritium as the mixed recombination rate (DT formation) is slightly higher than the tritium molecule recombination rate and slightly lower than the deuterium molecule recombination rate: $K_r^{D_2} > K_r^{DT} > K_r^{T_2}$ (Fig. 3).

Table 2
Data of adsorption and sticking coefficients for the deuterium interaction with MANET at different surface conditions

D$_2$/MANET	k_{ad} (molec. m^{-2} s^{-1} Pa^{-1})	Sticking factor at $T = 741$ K
Bare surface k_{ad}^{bare} [17]	$3.348 \times 10^{17} \exp(-0.198/kT)$	3.1×10^{-7}
Perfectly cleaned surface k_{ad}^{clean} [18,19]	$1.318 \times 10^{24}/\sqrt{T}$	1

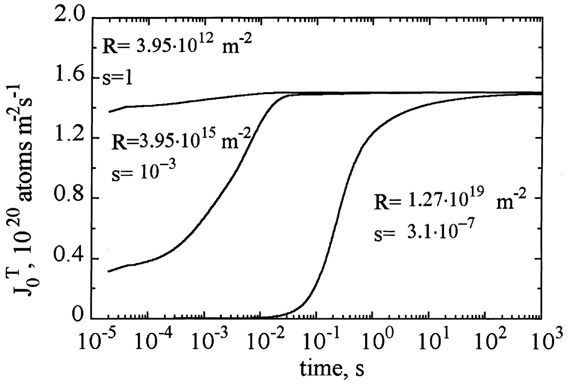

Fig. 1. Tritium re-emission rate for different sticking coefficients s on the plasma-facing side: $s=1$, perfectly clean surface; $s=10^{-3}$, corresponding 1 g/d of tritium permeation in the water coolant [22]; $s=3.1\times10^{-7}$, bare surface [17]. The corresponding recycling coefficient $R=D_iK_s^2/2\mu_i s$ is also given for comparison. The reflection component is not included.

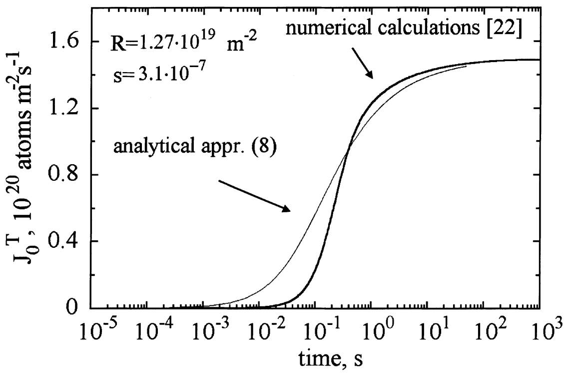

Fig. 2. Tritium re-emission flux as a function of time calculated for a bare steel surface $s=3.1\times10^{-7}$ by the model, Ref. [22], and by analytical approximation, Eq. (8).

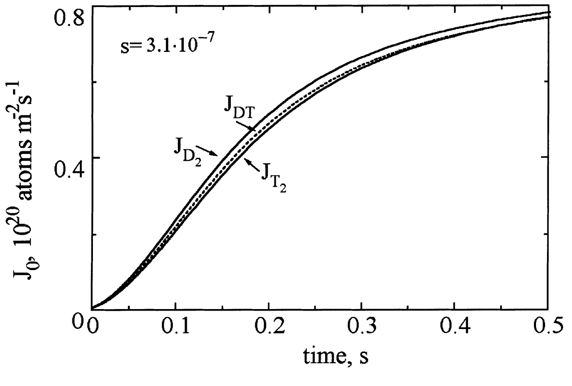

Fig. 3. Hydrogen isotope re-emission rate for a bare steel surface, $s=3.1\times10^{-7}$.

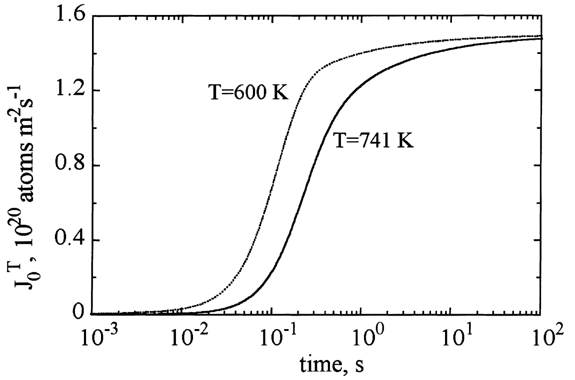

Fig. 4. Tritium re-emission rate at different temperatures of the FW calculated for a bare steel surface $s=3.1\times10^{-7}$.

3.3. Temperature effects

According to Ref. [21] the temperature of the plasma-facing side of the FW for the water-cooled Pb–17Li blanket is $T=741$ K. The reduction of the surface heat load decreases the FW temperature. As a result, the recombination coefficient $K_r\approx\exp(2(Q_s-E_c)/kT)$ increases due to $Q_s>E_c$ for F82H, that leads to a decrease of the time τ of the re-emission flux J_0 to reach saturation. Fig. 4 demonstrates that the reduction of the temperature T decreases τ.

3.4. Trapping effects

The trapping of ion-implanted hydrogen isotopes is usually dominated by vacancies for hydrogen isotope concentrations up to several atomic percent [23]. Ac-

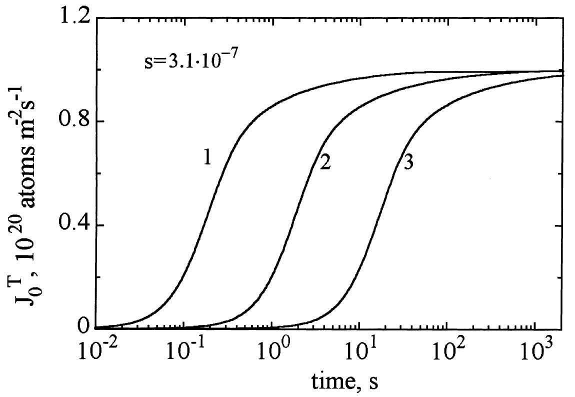

Fig. 5. Influence of neutron-produced defects on the tritium re-emission rate for a bare steel surface $s^{\mathrm{bare}}=3.1\times10^{-7}$. Curve 1 – without taking into account defects, curve 2 – taking into account neutron-generated defects with 0.1% of traps, and curve 3 – taking into account neutron-generated defects with 1% of traps. The trapping energy is $E_b=0.63$ eV.

cording to Ref. [24], the trap concentration of vacancies generated by neutron irradiation can be taken as 1 at.%. According to [20], the trap concentration caused by neutron irradiation is 0.1 at.%. In this work, the hydrogen isotope re-emission rate using both 1 and 0.1 at.% of traps has been calculated. The trap binding energy (derived from the difference in the potential energy of an atom in the normal position in solution and in the state of binding with the defect) is related to the vacancy trap type and can be taken as $E_b = 0.63$ eV [23,24]. Fig. 5 shows the influence of neutron-produced defects on the tritium re-emission rate. The trapping can delay the recycling time τ by more than two orders of magnitude.

4. Conclusions

Total recycling consists of two processes: reflection of implanted hydrogen isotopes from the first wall and re-emission due to surface recombination. In this work, the re-emission rate has been calculated. The factors which influence the re-emission rate are the sticking coefficient, the temperature of the plasma-facing side of the FW and trapping in neutron-induced defects. These factors influence only the time τ of the re-emission flux to reach the steady state but do not influence the value of the steady state re-emission flux. The increase of the sticking coefficient s (i.e. removing of the surface contamination) and the reduction of the temperature T on the plasma-facing side of the FW both reduce the recycling time τ. On the other hand, trapping in neutron-produced defects can increase τ by more than two order of magnitude.

According to Ref. [22] it should be mentioned that an increase of the sticking coefficient s leads to a decrease of the permeation flux and inventory. The decrease of the temperature on the front side of the FW also decrease the permeation flux and inventory because of the increase of the front recombination coefficient.

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