



# On hydrogen transport in the first wall material of fusion devices in the presence of a broadband distribution of traps over the trapping energy



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## ABSTRACT

The dynamics of hydrogen dissolved in a sample with continuous distribution of traps over trapping energy  $\varphi(\varepsilon) \propto \exp(-\alpha\varepsilon)$  ( $\varepsilon = E/T$  is the ratio of trapping energy  $E$  to the sample's temperature  $T$ ) is considered. Assuming that the hydrogen density is smaller than the trap density and the most of hydrogen is trapped, we found that the dynamics of hydrogen transport can be described by either sub-diffusion or non-linear diffusion equations. Analysis of the outgassing of the sample homogeneously loaded with hydrogen gives, in the most important cases, both power-law,  $\Gamma_H \propto t^{-p}$  ( $p \geq 1/2$ ) and exponential,  $\ln(\Gamma_H) \propto -t^\alpha$ , time dependencies of the outgassing flux,  $\Gamma_H(t)$ .

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## 1. Introduction

Tritium retention in the material of the first wall is one of the main issues for future fusion reactors (e.g. see Ref. [1] and the references therein). Therefore, it is important to understand the physics of retention caused by trapping of hydrogenic species in imperfections of material lattices (e.g. vacancies, impurities, grain boundaries, etc.).

In the studies of the hydrogen retention the modeling of hydrogen thermal desorption spectra (TDS) is the most common approach. Potentially such modeling can provide the information on both the trapping energies and amount of hydrogen trapped in different traps. Usually modeling is performed with 1D reaction-diffusion (RD) equations (which take into account hydrogen diffusion and trapping-detrapping processes) and proper boundary conditions at the surfaces (e.g. see Ref. [2] and the references therein). In most cases only two–three traps with different trapping energy are considered.

However, in fusion devices majority of retained hydrogen is accumulated in a co-deposited material [1,3,4]. This material contains a large amount of hydrogen and, probably, has amorphous-like structure, which may have traps characterized by a large variety of trapping energies. As a result, to describe hydrogen transport in and outgassing from co-deposits one should use large number of the RD equations. But in this case a more appropriate way for the

description of hydrogen transport could be based on a continuum kinetic model of the population of traps over activation energy (broadband distribution),  $E$ , assuming that detrapping energy spectrum,  $P_E(\varepsilon)$ , is known (here  $\varepsilon = E/T$ ,  $T$  is the wall temperature) [5]. We notice that recently similar broadband approach was suggested to use for the modeling of hydrogen retention in plasma facing components exposed to large fluence of 14 MeV neutrons [6], since standard methods were inadequate to fit experimental data. This is not surprising, since material damage associated with neutrons results in effective “amorphization” of material structure, which becomes somewhat similar to that in co-deposits.

In Ref. [5] it was shown that for the case of a broadband trap distribution the transport of a trace particle can be analyzed with the theory of random walk on a lattice with varying waiting time,  $\tau$ , given by the probability function,  $P_\tau(\tau)$  (e.g. see Ref. [7] and the references therein). This probability function can be expressed in terms of  $P_E(\varepsilon)$  as follows:  $P_\tau(\tau) = \int_0^\infty \{f(\tau/\tau_E)/\tau_E\} P_E(\varepsilon) d\varepsilon$ , where  $\tau_E = \tau_0 \exp(\varepsilon)$ ,  $\tau$  is the normalization constant, and the function  $f(\tau/\tau_E)$  describes the contribution to the waiting time distribution from one kind of traps with the energy  $E$ :  $P_\tau(\tau, E) = f(\tau/\tau_E)/\tau_E$ . For  $P_E(\varepsilon) = \alpha \exp(-\alpha\varepsilon)$  we find  $P_\tau(\tau \rightarrow \infty) \propto \tau^{-(1+\alpha)}$ , which for  $0 < \alpha < 1$  and the simple cubic lattice with size  $\ell$ , corresponds to the sub-diffusion process [7] resulting in a power-law time dependence of the outgassing flux:  $\Gamma_H(t) \propto t^{-(1-\alpha/2)}$ . Recalling recent results on the outgassing dynamics in JET and Tor Supra showing  $\Gamma_H(t) \propto t^{-0.7}$  [3,4], we can conclude that within our approach these experimental results can be explained with exponential trapping spectrum for  $\alpha = 0.6$  [5].

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For porous media, to which co-deposits might be attributed for, the effective step size  $\ell$  for a walker can also be random and described by the probability function  $P_\ell(\ell)$ . For the case where  $P_\ell(\ell \rightarrow \infty) \propto 1/\ell^{1+\beta}$  and  $1 < \beta < 2$  hydrogen transport will be impacted by Levi flights [8]. Combination of power-law distributions of waiting time ( $0 < \alpha < 1$ ) and step-size ( $1 < \beta < 2$ ) of a random walker results in a transport process, which can be described by partial fractional differential equation [8]

$$\frac{\partial^\alpha [H]}{\partial t^\alpha} = D_{\text{eff}} \frac{\partial^{2/(3-\beta)} [H]}{\partial t^{2/(3-\beta)}}, \quad (1)$$

where  $[H]$  is the hydrogen density and  $D_{\text{eff}}$  is the effective “diffusion” coefficient. We notice that partial fractional differential equations are used to describe transport phenomena in different areas of science including anomalous plasma transport in fusion devices [9,10].

Thus we see that the broadband distribution of traps over trapping energy results in much richer physics than the standard models with just two–three energy traps. However, in Ref. [5] only trace approximation of hydrogen in material was considered assuming that all traps are virtually unoccupied. In practice this is not the case. Therefore, in what follows we will analyze the impact of non-linear processes of hydrogen transport related to the occupation of traps with broadband energy distribution.

In Section 2 we derive hydrogen transport equation for  $P_E(\varepsilon) = \alpha \exp(-\alpha\varepsilon)$ . In Section 3 we consider different analytically tractable limits of this equation. In Section 4 we derive the expressions for the time dependence of hydrogen outgassing flux  $\Gamma_H(t)$  in different regimes and in Section 5 we summarize our main conclusions.

## 2. Hydrogen transport equations for continuous distribution of traps over trapping energy

We assume that there stationary and homogeneous continuous distribution of traps over trapping energy, which is described by the distribution function  $\varphi(\varepsilon)$ , so that the trap's density can be expressed as  $N_{\text{tr}} = \int \varphi(\varepsilon) d\varepsilon$ , where  $\varepsilon = E/T$  is the ratio of trapping energy  $E$  to the sample's temperature  $T$ . The population of these traps with hydrogen we will describe with the distribution function  $f(\varepsilon, \vec{r}, t)$ , so that the density of trapped hydrogen,  $n_{\text{tr}}(\vec{r}, t)$ , is  $n_{\text{tr}}(\vec{r}, t) = \int f(\varepsilon, \vec{r}, t) d\varepsilon$ . Then the reaction–diffusion equations with continuous trap distribution can be written as follows:

$$\frac{\partial n_{\text{tr}}}{\partial t} = D \nabla^2 n_{\text{tr}} - d\varepsilon \{ K_{\text{tr}} n_{\text{tr}} (\varphi - f) - \nu_{\text{dt}}(\varepsilon) f \}, \quad (2)$$

$$\frac{\partial f}{\partial t} = K_{\text{tr}} n_{\text{tr}} (\varphi - f) - \nu_{\text{dt}}(\varepsilon) f, \quad (3)$$

where  $n_{\text{fr}}(\vec{r}, t)$  is the density of free hydrogen,  $K_{\text{tr}}$  and  $\nu_{\text{d}}(\varepsilon) = \hat{\nu}_{\text{d}} \exp(-\varepsilon)$  are correspondingly the rate constant and frequency of hydrogen trapping and detrapping processes (here  $\hat{\nu}_{\text{d}}$  is the normalization constant and we assume that  $K_{\text{tr}}$  does not depend on  $\varepsilon$ ). We notice that Eq. (2) or Eq. (3) can be substituted with the equation describing the balance of total hydrogen density,  $N_{\text{H}} = n_{\text{fr}} + n_{\text{tr}}$ :

$$\frac{\partial N_{\text{H}}}{\partial t} = D \nabla^2 n_{\text{fr}}. \quad (4)$$

We will consider the solution of Eqs. (2)–(4) aimed on hydrogen outgassing from the sample under some assumptions:

- (i) The density of free hydrogen is smaller than the trapped one,

$$N_{\text{H}} \approx n_{\text{fr}} \gg n_{\text{tr}}, \quad (5)$$

since the opposite case, taking into account Eq. (4), is trivial;

- (ii) Hydrogen density is much smaller than the density of traps,  $N_{\text{H}} < N_{\text{tr}}$ ,

$$N_{\text{H}} < N_{\text{tr}}. \quad (6)$$

- (iii) Trap density is relatively small, so that

$$\nu_{\text{tr}} \equiv K_{\text{tr}} N_{\text{tr}} < \hat{\nu}_{\text{d}}. \quad (7)$$

- (iv) The scale length of hydrogen density variation,  $\Delta$ , and, therefore, effective diffusion time of free hydrogen,  $\tau_{\Delta} \sim \Delta^2/D$ , are large enough so that retrapping of free hydrogen is vital for the hydrogen dynamics:

$$\nu_{\text{tr}} \tau_{\Delta} > 1. \quad (8)$$

In opposite case hydrogen flux will be simply determined by the detrapping process of initial distribution of trapped hydrogen.

If we ignore the impact of free hydrogen diffusion, than the system (2), (3) will approach with time the equilibrium distribution function

$$f_{\text{eq}}(\varepsilon) = \varphi(\varepsilon) \frac{K_{\text{tr}} n_{\text{fr}}}{K_{\text{tr}} n_{\text{fr}} + \nu_{\text{d}}(\varepsilon)}, \quad (9)$$

which gives the following relation between free and trapped hydrogen densities for equilibrium condition:

$$(n_{\text{tr}})_{\text{eq}} = \int f_{\text{eq}}(\varepsilon) d\varepsilon \equiv d\varepsilon \frac{\varphi(\varepsilon) K_{\text{tr}} n_{\text{fr}}}{K_{\text{tr}} n_{\text{fr}} + \nu_{\text{d}}(\varepsilon)}. \quad (10)$$

In general case from Eq. (3) we find a formal solution for the distribution function

$$f = f_0 \exp\{-(K_{\text{tr}} \eta(t) - \nu_{\text{d}} t)\} + \int_0^t dt' \varphi K_{\text{tr}} \frac{d\eta(t')}{dt'} \times \exp\{-[K_{\text{tr}}(\eta(t) - \eta(t')) - \nu_{\text{d}}(t - t')]\}, \quad (11)$$

where

$$\eta(t) = \int_0^t n_{\text{fr}}(t') dt' \quad \text{and} \quad f_0(\varepsilon, \vec{r}) \equiv f(\varepsilon, \vec{r}, t = 0). \quad (12)$$

To proceed any further we need to specify the function  $\varphi(\varepsilon)$ . In what follows, we will assume that

$$\varphi(\varepsilon) = \alpha N_{\text{tr}} \exp(-\alpha\varepsilon), \quad (13)$$

where  $\alpha$  is an adjustable parameter. Recalling that the variable  $\varepsilon$  is the ratio of trapping energy  $E$  to the sample's temperature  $T$ , such choice for  $\varphi(\varepsilon)$  looks quite natural. To describe the cases where sample's temperature varies in time we can adopt a proper time variation of  $\alpha = \alpha(t)$ . However, in this study we will assume  $\alpha = \text{const}$ . Recall that in Ref. [5] it was shown that in the linear approximation (neglecting the term  $\propto n_{\text{fr}} f$  in the right-hand side of Eqs. (2), (3)) such choice of  $\varphi(\varepsilon)$  with  $\alpha < 1$  describes a random walk with a power-law waiting time distribution resulting in a sub-diffusion process.

By using Eq. (13) we find that for the equilibrium condition we have the following relation between free and trapped hydrogen densities

$$(n_{\text{tr}})_{\text{eq}} = N_{\text{tr}} \left( \frac{K_{\text{tr}} n_{\text{fr}}}{\hat{\nu}_{\text{d}}} \right)^\alpha \int_0^{(\hat{\nu}_{\text{d}}/K_{\text{tr}} n_{\text{fr}})^\alpha} \frac{d\xi}{1 + \xi^{1/\alpha}}. \quad (14)$$

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