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Effect of transport on MAR in detached divertor plasma

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Abstract

The effect of H_2 transport on the onset of MAR in the relatively lower plasma parameter regime of a detached state ($n_e = 1 \times 10^{19}$ m^{-3}, $T_e = 1$ eV) is investigated theoretically. The vibrationally excited molecular densities and the degree of MAR are evaluated by using a 1-D Monte Carlo method (with transport effect), and by solving time-dependent 0-D rate equations without the transport term (without transport effect), respectively. It is found that the degree of MAR with transport is smaller than that without transport under the same H_2 flow rate. Especially, the degree of MAR is negligible near the gas inlet. This smaller degree of MAR with transport is due to the lack of highly excited vibrational molecules which contribute to MAR. The hydrogen molecular density available for MAR is determined by the external hydrogen molecular source and the outflow due to transport, i.e., a 'net' confinement time.

Keywords: Detached divertor plasma; MAR; Vibrationally excited state hydrogen molecule; Neutral transport; H_2 flow rate; Confinement time

1. Introduction

The reduction of heat load and particle influx onto a divertor plate is one of the critical issues to realize steady state or long pulse operation in magnetic fusion reactors. The detached plasma operation mode [1–3] is considered to be a promising candidate for the achievement of this requirement. The detached state is characterized by the simultaneous decrease of electron temperature and density, low heat load and decrease of ion influx toward the divertor plates.

The volume recombination process is one of the reasons for the reduction of the ion influx onto the divertor plates. Especially the molecular activated recombination (MAR) has been predicted to enhance the recombination rate in many theoretical models [4,5]. It is considered that MAR consists of two channels; (i) negative ion production: $H_2(v) + e \rightarrow H^- + H$, followed by $H^- + H^+ \rightarrow 2H$, and (ii) molecular ion production: $H_2(v) + H^+ \rightarrow H_2^+ + H$, followed by $H_2^+ + e \rightarrow 2H$. The effect of MAR has been verified in the linear machine, NAGDIS-II [6]. However, the effect of MAR has not been observed clearly in tokamaks [7].

The discrepancies between theories and tokamak experiments, or experimental results obtained with different types of devices are due to underlying parameters essential for the effect of MAR such as the plasma density and temperature, the hydrogen molecular source, and the confinement times of ions and neutrals. Thus, it is important for a comprehensive explanation of MAR to clarify the conditions under which MAR becomes effective.

For the relatively higher plasma parameter regime ($n_e > 1.0 \times 10^{20}$ m^{-3}, $T_e \sim$ a few eV), it is reported that the effect of the re-ionization of excited atoms and the conversion of H_2^+ into $H^+ + H$ are essential processes for the onset of MAR [8,9]. This physical mechanism explains well the reason why the onset of MAR does not appear in tokamaks.

On the other hand, for the relatively lower plasma parameter regime in a linear machine ($n_e \sim$ an order of 10^{19} m^{-3}, $T_e \leqq 1$ eV), it has been recently reported that

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the H_2 flow rate plays an important role for the transition from electron-ion recombination to MAR in the volume recombination process [10]. The relation between the H_2 flow rate and the onset of MAR is also pointed out in Ref. [11].

The H_2 flow rate corresponds to a hydrogen molecular source. In the particle conservation of hydrogen molecules, the outflow during transport should be simultaneously taken into account. In order to clarify the MAR physics in the relatively lower plasma parameter regime, we investigate the effect of hydrogen molecular transport on the onset of MAR. In relation to the transport effect, the correlation between the H_2 flow rate and the onset of MAR is also reported in this paper.

2. Numerical model

The rate equations for vibrationally ground and excited state molecules are generally given by

$$\frac{\partial}{\partial t} n_{H_2}(v) = S(v) + \Gamma_{in} - \Gamma_{out}. \quad (1)$$

The term $S(v)$ is the source/sink due to atomic and molecular processes. The term Γ_{in} is the molecular source which is externally introduced by gas puffing, while the term Γ_{out} corresponds to the outflow of molecules by their transport. Two cases with/without the transport term Γ_{out} are compared to investigate the effect of molecular transport on the onset of MAR.

The spatial distributions of $H_2(v)$ densities and the recombination rate due to MAR are numerically evaluated by using a Monte Carlo method [12] for the case with transport. From the assessment of the relaxation times of the population ($\sim$60 μs for $n_e = 1.0 \times 10^{19}$ m^{-3}, $T_e = 1$ eV) and the residence time ($\sim$100 μs), the trajectories of each vibrationally excited molecule are followed separately [13,14]. An illustration of the calculation model is shown in Fig. 1. A simple one-dimensional flow direction is modeled. Thus, hydrogen molecules are introduced from the one side and flowed out of the other side. As for the vibrationally excited

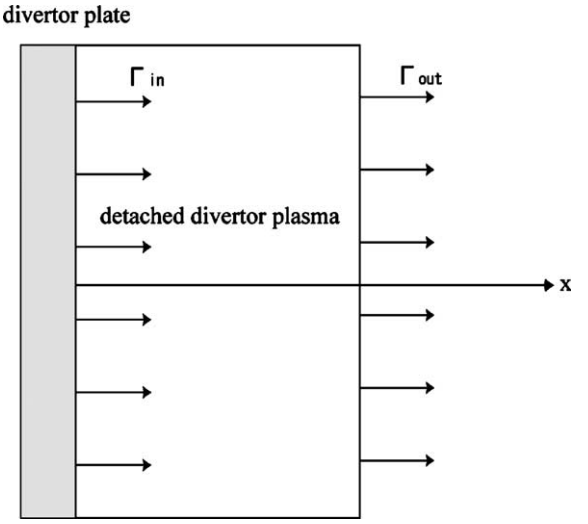

Fig. 1. An illustration of the calculation model. The term Γ_{in} is the molecular source which is externally introduced by gas puffing, while the term Γ_{out} corresponds to the outflow of molecules by their transport.

molecular source term Γ_{in}, hydrogen molecules in the vibrationally ground state are assumed to be provided by gas puffing. The vibrationally excited state molecules are generated from the vibrationally ground state by electron impact excitation/de-excitation. The vibrationally excited molecules are assumed to move with the velocity of room temperature. As a typical lower plasma parameter regime of the detached state, the plasma density and the plasma temperature are taken to be 1×10^{19} m^{-3} and 1 eV, respectively. The atomic and molecular processes taken into account in the present model are listed in Table 1. The excitation and de-excitation of $H_2(v)$ through excitation to the electronically excited states are not taken into account since this process is negligible in the low electron energy region (electron energy < 12 eV) [15].

The vibrationally excited molecular densities without transport are evaluated by directly solving the rate

Table 1
Atomic and molecular processes included in the present model

Processes	Reaction formulae
1. Excitation/de-excitation ($\Delta v = 1$)	$e + H_2(v) \rightarrow e + H_2(v+1)$
2. Dissociation	$e + H_2(X^1\Sigma_g^+) \rightarrow e + H_2 * (b^3\Sigma_u^+, a^1\Sigma_g^+,$ and $c^1\Pi_u) \rightarrow e + H(1s) + H(1s)$
3. Ion conversion	$H_2(v) + H^+ \rightarrow H_2^+(v) + H(1s)$
4. Dissociative attachment	$H_2(v) + e \rightarrow H^- + H$
5. Mutual neutralization	$H^- + H^+ \rightarrow H(n=2) + H(1s)$
	$H^- + H^+ \rightarrow H(n=3) + H(1s)$
6. Dissociative recombination	$H_2^+(v) + e \rightarrow H(1s) + H(n)$
7. Electron impact detachment	$H^- + e \rightarrow H(1s) + e + e$

The data is obtained from Refs. [18,19].

equation (1) without the transport term Γ_{out}. The initial H^+ density is assumed to be equal to the initial electron density. As for the H_2 source term Γ_{in}, the hydrogen molecules in the vibrationally ground state are assumed to be provided by gas puffing, which is similar to the case with transport. In the present calculations, the initial H_2 density is set to be zero. Thus, the vibrationally excited state molecules are generated from the vibrationally ground state by electron impact excitation/de-excitation. The numerical solutions are obtained by using Gear's method.

3. Results and discussion

To quantify the degree of MAR, we define the enhancement factor of the recombination rate by $(\nu_{\text{MAR}} + \nu_{R+3})/\nu_{R+3}$, where ν_{MAR} is the recombination rate due to MAR and ν_{R+3} is due to radiative and three-body recombination. The rate coefficients of radiative and three-body recombination are taken from Ref. [16].

The effect of the re-ionization of excited atoms as described in Section 1 were examined prior to the present analysis. We verify that this re-ionization effect is quite small as far as the present calculation condition is concerned. Whether the re-ionization of the excited atoms becomes effective or not strongly depends on the plasma parameter regime. The details will be reported elsewhere.

The spatial distributions of this enhancement factor with/without H_2 transport are shown in Fig. 2. The flow rate of hydrogen molecules for the case without transport is determined to become the ratio $n_{H_2}/n_e \sim 0.1$ in the quasi-steady state, where n_{H_2} is the sum of densities of the vibrationally ground and all excited states, i.e., $n_{H_2} \equiv \sum_{v=0}^{14} n_{H_2(v)}$. As for the case with transport, the following two cases of the flow rates are investigated:

Case I flow rate $= 4.2 \times 10^{20}$ s^{-1} (this value is the same as that without transport).
Case II flow rate $= 1.1 \times 10^{21}$ s^{-1} (the ratio n_{H_2}/n_e is the same as that without transport).

The enhancement factor is evaluated to be 8.7 without transport. Moreover, the channel through negative ion production is dominant in MAR. In Ref. [4], it is reported that (i) the enhancement factor is estimated to be 30, and (ii) the dominant channel of MAR is molecular ion production rather than negative ion production. This discrepancy is caused by the smaller rate coefficient of ion conversion due to the lower H_2 energy in the present model. In fact, both the enhancement factor and the dominant channel of MAR are in good agreement with Ref. [4] when the H_2 energy is 1 eV.

In spite of the same flow rate, the enhancement factor for case I is less than half of the enhancement factor without transport all over the calculation region. In particular, the enhancement factor is approximately 1 near the gas inlet, which means that the effect of MAR is negligible. For case II, the enhancement factor is larger than for case I. Although the effect of MAR is also negligible near the gas inlet, the enhancement factor far from the gas inlet is as much as the value without transport.

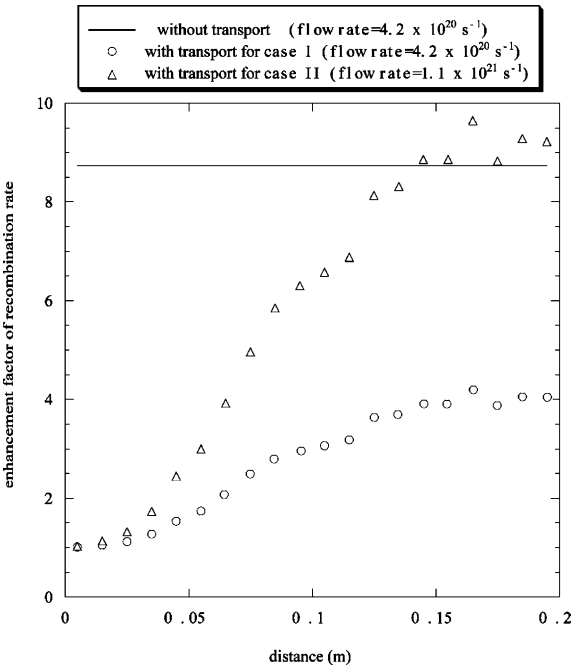

Fig. 2. The spatial distributions of the enhancement factors of recombination due to MAR with/without H_2 transport are compared. For the spatial distribution H_2 with transport, two cases of H_2 flow rate are shown: The H_2 flow rate is the same as that without transport for case I, while the ratio n_{H_2}/n_e is the same as that without transport for case II.

The spatial distributions of $H_2(v)$ densities with/without H_2 transport are shown in Fig. 3. The vibrationally excited hydrogen molecular densities with transport are much smaller than those without transport near the gas inlet. The negative ion production efficiency, i.e., MAR is mainly contributed from high vibrational states ($v \geqq 6$). Therefore, the reason why the effect of MAR is scarcely appeared near the gas inlet with transport is the lack of highly excited vibrational molecules. The vibrationally excited molecular densities increase away from the gas inlet through excitation/de-excitation by electron impact, whereas the ground state molecular density decreases. However, the vibrationally excited molecular densities are one-third as large as the densities without transport. These smaller vibrationally excited molecular densities result in the smaller effect of MAR away from the gas inlet for case I.

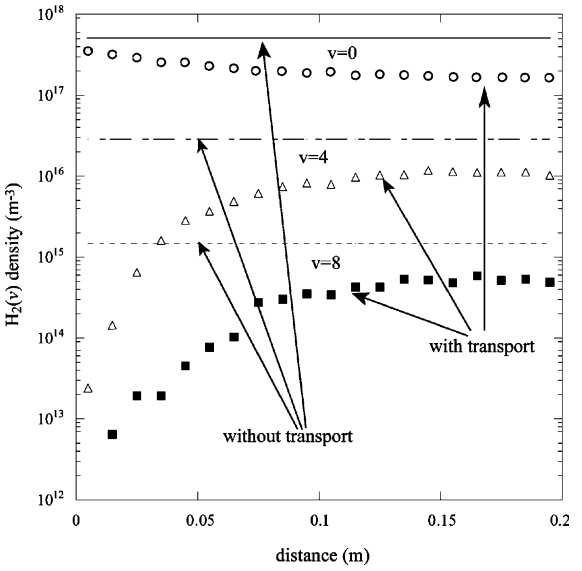

Fig. 3. The spatial distributions of $H_2(v)$ densities with/without H_2 transport are compared for case I in Fig. 2. The $H_2(v)$ densities for the vibrational states $v = 0$ (ground state), 4, 8 are shown in this figure.

The relation between the hydrogen molecular density available for MAR and the transport effect can be explained as follows: the transport term Γ_{out} is given by $\Gamma_{\text{out}} = n_{H_2}(v)/\tau$, where τ is the confinement time of hydrogen molecules. In the quasi-steady state, the sum of Eq. (1) over all the vibrational levels leads to

$$0 \sim -\sum_v \{S_{\text{DA}}(v) + S_{\text{IC}}(v) + S_{\text{diss}}(v)\} n_{H_2}(v) n_e + \Gamma_{\text{in}} - \frac{n_{H_2}}{\tau}, \quad (2)$$

where S_{DA}, S_{IC}, and S_{diss} are the rate coefficients of dissociative attachment, ion conversion, and molecular dissociation, respectively. Let us define the average sink due to these collisional processes as

$$(\sin k)_{\text{av}} \equiv \frac{\sum_v \{S_{\text{DA}}(v) + S_{\text{IC}}(v) + S_{\text{diss}}(v)\} n_{H_2}(v) n_e}{n_{H_2}}. \quad (3)$$

By substituting Eq. (3) into Eq. (2), we obtain

$$n_{H_2} = \frac{\Gamma_{\text{in}}}{(\sin k)_{\text{av}} + 1/\tau}. \quad (4)$$

It is explicitly shown in Eq. (4) that the hydrogen molecular density available for MAR depends on the source term Γ_{in} and the confinement time. The hydrogen molecular density becomes smaller by a factor of $1/\tau$ due to the transport effect. The value of $(\sin k)_{\text{av}}$ is estimated to be 1–2 $\times 10^3$ s^{-1} under the present calculation conditions. On the other hand, the value of $1/\tau$ is estimated to be $\sim 1/(0.2\ \text{m}/1.1 \times 10^3\ \text{m/s}) = 5.6 \times 10^3\ s^{-1}$ on the assumption that hydrogen molecules move with the velocity of room temperature. Therefore, the transport effect on the hydrogen molecular density is remarkable. It is also suggested by Eq. (4) that the amount of H_2 flow rate should be increased to make MAR become effective. This is apparent from the comparison of the enhancement factor of the recombination rate between the case I and the case II as shown in Fig. 2.

4. Summary and future plan

We focus our study on the neutral transport effect as one of the important parameters for the onset of MAR under the relatively low plasma parameter regime ($n_e \sim$ an order of 10^{19} m^{-3}, $T_e \leqq 1$ eV). The effect of hydrogen molecular transport on the onset of MAR is investigated theoretically. The vibrationally excited molecular density and the recombination rate due to MAR are evaluated by using a Monte Carlo method (for the case with transport) and solving time-dependent 0-D rate equations (for the case without transport). A simple 1-D flow direction is modeled for the case with transport. It is found that the degree of MAR with transport is smaller than that without transport under the same H_2 flow rate. Especially, the degree of MAR is negligible near the gas inlet. This difference in the degree of MAR is attributed to the hydrogen molecular density in high vibrational states. The hydrogen molecular density available for MAR is determined by the both the external hydrogen molecular source and the outflow due to transport, i.e., a 'net' confinement time of hydrogen molecules. Therefore, the onset of MAR cannot appear if an amount of the H_2 source is not enough to compensate the outflow of hydrogen molecules. The reason why the onset of MAR strongly depends on the H_2 flow rate in a linear device seems to be the net confinement time of hydrogen molecules. For comparison with experimental results, it is required to model neutral transport in more detail. For example, in the present model, hydrogen molecules are assumed to be provided in the ground state. However, it is reported that hydrogen molecules are desorbed in the vibrationally excited states from the surface of tungsten [17] which is used as a material of the divertor plate. Improvement of the neutral transport model will be carried out in the future.

References

[1] B. LaBombared et al., J. Nucl. Mater. 241–243 (1997) 149.
[2] A. Loarte, R. Monk, J.R. Martin-Solis, et al., Nucl. Fus. 38 (1998) 331.
[3] H. Tamai, N. Asakura, N. Hosogane, J. Plasma and Fus. Res. 74 (1998) 1336.

[4] S.I. Krasheninnikov, A.Yu. Pigarov, D.J. Sigmar, Phys. Lett. A 214 (1996) 295.
[5] A.Yu. Pigarov, S.I. Krasheninnikov, Phys. Lett. A 222 (1996) 251.
[6] N. Ohno, N. Ezumi, S. Takamura, et al., Phys. Rev. Lett. 81 (1998) 818.
[7] R.C. Isler, G.R. Mckee, N.H. Brooks, et al., Phys. Plasmas 4 (1997) 2989.
[8] D. Reiter, Chr. May, M. Baelmans, P. Borner, J. Nucl. Mater 241–243 (1997) 342.
[9] U. Fantz, D. Reiter, B. Heger, D. Coster, J. Nucl. Mater. 290–293 (2001) 367.
[10] N. Ohno, D. Nishijima, S. Takamura, et al., Nucl. Fus. 41 (2001) 1055.
[11] K. Miyamoto, A. Hatayama, Y. Ishii, et al., Contrib. Plasma Phys. 42 (2002) 333.
[12] D. Heifetz, D. Post, M. Petravic, J. Weisheit, G. Bateman, J. Comput. Phys. 46 (1982) 309.
[13] K. Miyamoto, Y. Ishii, A. Hatayama, to be published in J. Appl. Phys.
[14] M. Uematsu, T. Morishita, A. Hatayama, et al., Rev. Sci. Instrum. 71 (2000) 883.
[15] K. Sawada, T. Fujimoto, J. Appl. Phys. 78 (1995) 2913.
[16] L.C. Johnson, E.J. Hinnov, J. Quant. Spectrosc. Radiat. Trans. 13 (1973) 333.
[17] R.I. Hall et al., Phys. Rev. Lett. 60 (1988) 337.
[18] R.K. Janev, W.D. Langer, K. Evance, D.E. Post, Elementary Processes in Hydrogen–Helium Plasmas, Springer-Verlag, Berlin, 1987.
[19] P.T. Greenland, D. Reiter, The role of molecular hydrogen in plasma recombination, JUEL-3528; Juelich report, Forshungszentrum Juelich (1996).