Redeposition Characteristics of Heavy Hydrocarbon Molecules on a Divertor Plate*)

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In this study, local redeposition characteristics of hydrocarbon molecules from the ethane family are investigated using Monte Carlo simulation. Information about redeposition characteristics is required to estimate tritium retention via redeposition with chemically eroded hydrocarbon molecules. For the condition of multiple reflections at divertor surface and a plasma density of $1.0 \times 10^{19}\,m^{-3}$, the local redeposition characteristics for injection of ethane family (C_2H_2, C_2H_4, C_2H_6) have been investigated for plasma temperatures ranging from 1 to 100 eV. The number of redeposited hydrocarbon molecules increases with plasma temperature because of the increase in impinging particle energy. The increase in sheath potential results in the increase in particle energy. For plasma temperatures lower than 5 eV, there is a sudden increase in the number of redeposited particles with plasma temperature because of the increase in the number of impinging molecular ions. Sheath field acceleration is the main mechanism that causes the ions to move to the divertor plate, and the exponential increase in the number of redeposited particles results from the increase in hydrocarbon break-up products in the sheath potential region.

Keywords: plasma-wall interaction, chemical erosion, hydrocarbon, computer simulation

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1. Introduction

In various magnetic confinement fusion devices, materials for the divertor plate and vacuum vessel wall are mostly carbon based. For safe and steady-state operations with tritium in advanced magnetically confined fusion devices, such as International Thermonuclear Experimental Reactor (ITER), estimation of tritium retention via tritium redeposition with chemically eroded hydrocarbon molecules is one of the most crucial plasma-wall interaction issues. Chemically eroded hydrocarbon compounds are generally dominated by methane; however, these compounds contain heavier hydrocarbons, e.q., ethane (C_2H_x) and propane (C_3H_x) species. These heavy hydrocarbons account for up to 50% of the total number of chemically eroded species at low incident energy [1]. Thus, chemically eroded ethane and propane families should be considered in the estimation of tritium retention. In previous studies, redeposition profiles and characteristics of CH_4 [2] and of C_2H_4 and C_2H_6 [3] were investigated using a simple model for divertor plasma region (constant plasma temperature and density). Further, in Ref. 3, poloidal distributions of redeposited carbons/hydrocarbons on the divertor surface were calculated. However, characteristics of redeposition species have not been discussed yet, and investigations of these characteristics are necessary to reveal the process of tritium retention caused by redeposition of tritiated hydrocarbon molecules. In this study, transport of heavy hydrocarbon molecules from the ethane family (acetylene:C_2H_2, ethylene:C_2H_4, ethane:C_2H_6) in a modeled tokamak divertor plasma is investigated using Monte Carlo simulation, and the redeposition characteristics of each hydrocarbon molecule are reported.

2. Simulation Model

In this study, the local redeposition characteristics of heavy hydrocarbon molecules in the modeled tokamak divertor plasma region are investigated using Monte Carlo simulation [2]. The divertor surface is assumed to be amorphous carbon. The following complex dissociation and the ionization reactions of hydrocarbon molecules are considered: (a) ionization and dissociative ionization by electron collision, (b) dissociation by electron collision, (c) dissociative recombination, and (d) charge exchange with hydrogen ions and surface reflection processes. The model includes 700 reactions, and the rate coefficients for molecular processes are taken from data-set of Janev and Reiter [4, 5]. The considered dissociation products are CH_x ($x \leq 4$), C_2H_x ($x \leq 6$), C_3H_x ($x \leq 8$), carbon, and carbon

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ions. The reflection coefficients for all dissociation products on an amorphous carbon surface were calculated by classical molecular dynamics [3]. Hydrocarbon molecular ions are produced by a reaction with ionization processes, and they gyrate because of the Lorentz force and move along the direction parallel to the magnetic field line because of the force $F_{\parallel}$. The parallel force $F_{\parallel}$ consists of friction force and thermal gradient force. The friction force is directed toward the divertor plate because the plasma flow is assumed to have no reversal flow in the simulation. The friction force increases with plasma density. The thermal gradient force causes ions to move upstream and increases with plasma temperature.

Incident energy of hydrocarbon molecules to the divertor plate plays a crucial role in the redeposition process, because the reflection coefficient strongly depends on the incident particle energy. One of the main mechanisms determining the incident particle energy is acceleration by an electric field. The electric field is divided into three components: sheath field, a parallel electric field along the magnetic field line, and a radial electric field. However, in this study, because the sheath field is considerably greater than the parallel and radial fields, we consider only the sheath field in the simulation model. The sheath field accelerates the hydrocarbon molecular ions toward the divertor plate. The sheath field is caused by the sheath potential $\Phi_s \approx 3T_e$. The sheath potential consists of the electric sheath $\Phi_{es} = \Phi_s f_D$ and the magnetic presheath $\Phi_{mps} = \Phi_s(1 - f_D)$ [6]. The Brooks parameter f_D is assumed to be 0.25 in this model. The spatial distribution of the sheath potential is given by

$$\Phi_s(z) = \Phi_{es} \exp\left(\frac{-z}{2\lambda_D}\right) + \Phi_{mps} \exp\left(\frac{-z}{R_L}\right), \qquad (1)$$

where z is the distance normal to the divertor surface, λ_D is the Debye length, and R_L is the Larmor radius of the plasma ions. Φ_{es} and Φ_{mps} rapidly decrease with increasing z. The widths of the electrostatic sheath and the magnetic presheath are of the order of 10 μm and 1 mm, respectively.

The simulation volume, which has constant plasma temperature and density, is $10 \times 10 \times 10\,\mathrm{cm}^3$, and the surface area of the divertor plate is $10 \times 10\,\mathrm{cm}^2$. The angle of the magnetic field lines with the toroidal direction is 5° and the lines are inclined by 30°. The magnetic field strength is 5 T. The heavy hydrocarbon molecules, ethane family (C_2H_2, C_2H_4, C_2H_6), are launched from the center of the divertor plate with Maxwellian velocity distribution corresponding to a temperature of 0.1 eV (1160 K). The number of released particles is 10^5. The transport of a launched hydrocarbon molecule is calculated until the molecule leaves the simulation volume or redeposits on the divertor surface. The simulation volume of $10 \times 10 \times 10\,\mathrm{cm}^3$ may not be sufficiently large for simulating long-range transport. For long-range transport, it is necessary to consider the curvature of the magnetic field and the divertor plate in the simulation model. Consequently, we focus on the local redeposition characteristics of hydrocarbon molecules. The simulation model is described in detail in Ref. 2. For the condition of multiple reflections at the divertor surface and a plasma density of $1.0 \times 10^{19}\,\mathrm{m}^{-3}$, the calculations have been performed for plasma temperatures ranging from 1 to 100 eV.

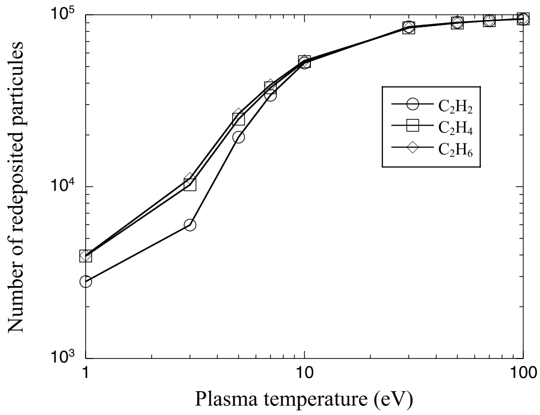

Fig. 1 Total number of redeposited particles in terms of plasma temperature for injection of C_2H_2, C_2H_4, and C_2H_6.

3. Results and Discussion

Figure 1 shows the total number of redeposited particles in terms of plasma temperature for the injection of C_2H_2, C_2H_4, and C_2H_6. The peak positions of the distributions of redeposited hydrocarbons are almost at the center of the surface, i.e., the injection point (the distance from the injection point is less than 1.5 mm). The e-holdings of redeposition distribution profiles are typically less than 2.5 mm. For example, for the injection of C_2H_4, the e-holdings of the C_2H redeposition profile at the plasma temperatures of 1 and 50 eV are 2.3 and 1.5 mm, respectively. The e-holdings of the C_2H^+ redeposition profile at the plasma temperatures of 1 and 50 eV are 1.8 and 1.3 mm, respectively. In Fig. 1, the total numbers of redeposited particles for the injection of C_2H_2, C_2H_4, and C_2H_6 at the plasma temperature of 1 eV are 2804, 3944, and 3974, respectively. These values increase with plasma temperature until the temperature reaches approximately 30 eV, and then they remain practically constant. The peak values of the total number of redeposited particles for each injection species are approximately 9.5×10^4. There are sudden increases in the total number of redeposited particles at low plasma temperatures (≤ 5 eV). More detailed research on the plasma temperature dependence of the total number of redeposited particles is needed to clarify the mechanisms that cause hydrocarbon molecular redeposition at low plasma temperatures.

Figures 2, 3, and 4 show the number of ionized and neutral species redeposited on the simulation surface (divertor plate) following the release of 10^5 C_2H_2, C_2H_4, and C_2H_6 molecules, respectively. For each injection species, carbon ions ($C^+ - C^{6+}$) are the dominant redeposited species at plasma temperatures higher than 5 eV.

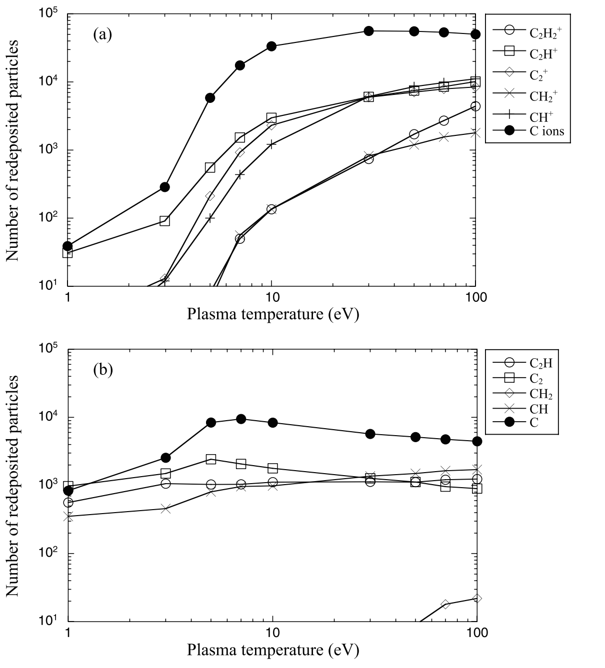

Fig. 2 Number of redeposited (a) ionized and (b) neutral species following the release of 10^5 C_2H_2 molecules.

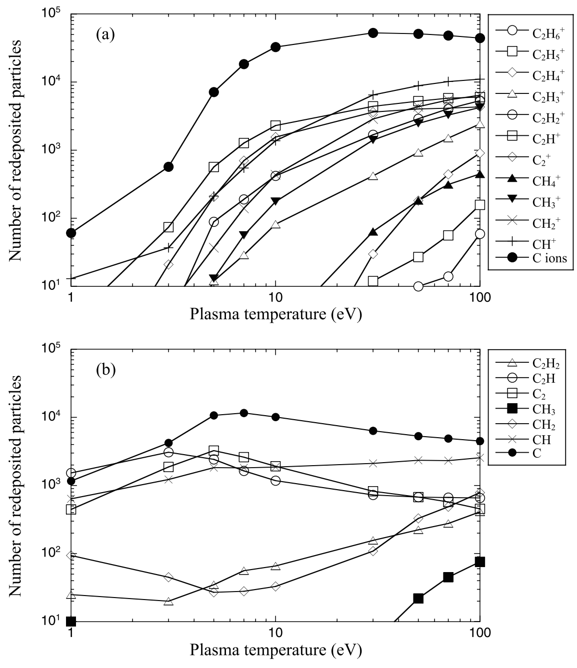

Fig. 4 Number of redeposited (a) ionized and (b) neutral species following the release of 10^5 C_2H_6 molecules.

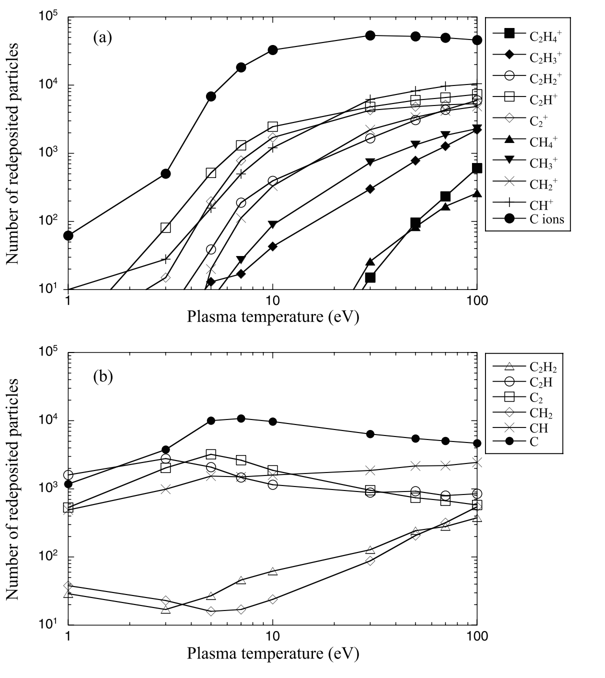

Fig. 3 Number of redeposited (a) ionized and (b) neutral species following the release of 10^5 C_2H_4 molecules.

At plasma temperatures lower than 5 eV, the carbon atom is the dominant redeposited species.

The number of redeposited hydrocarbon molecular ions increases with plasma temperature. The main redeposited species of hydrocarbon molecular ions are CH^+, CH_2^+, CH_3^+, and C_2H^+ at plasma temperatures ranging from 5 to 100 eV. The number of redeposited ions are on the order of $10^3 \sim 10^4$ at the plasma temperature of 100 eV. For example, for the injection of C_2H_2, the numbers of redeposited CH_2^+ and C_2H^+ at the plasma temperature of 100 eV are 1799 and 10138, respectively. On the other hand, at plasma temperatures lower than 5 eV, the number of redeposited ions is considerably small. For example, for the injection of C_2H_2, the number of redeposited C_2H^+ ranges from 31 to 2979.

The main redeposited species of hydrocarbon molecules are C_2H_2, C_2, and C. For the injection of C_2H_2 (Fig. 2 (b)), the number of these molecules equalizes in terms of the plasma temperature. For the injection of C_2H_4 and C_2H_6 (Figs. 3 (b) and 4 (b)), the redeposition of CH_2 and C_2H_2 are observed. The number of redeposited species decreases slightly with increasing plasma temperature until the temperature reaches approximately 5 eV, and then it increases with plasma temperature.

As shown in the figures, the number of redeposited hydrocarbon molecular ions increases with plasma temperature. This dependence is due to the plasma temperature dependence of (a) reflection and (b) atomic and molecular processes. In the reflection process, a reflection coefficient is important to determine the motion of the particles after they impinge on the divertor surface, i.e., reflection or redeposition. The reflection coefficients considered in this study are shown in Fig. 5 [3]. In Fig. 5, the reflection coefficients decrease with increasing particle energy because of the increase in the penetration depth in the bulk of the hydrogenated and amorphized carbon surface. In the edge plasma region, the main mechanism for determining the incident energy of hydrocarbon molecular ions is sheath acceleration. The sheath potential is proportional to the electron temperature, and thus the incident energy of hydrocarbon molecular ions increases with increasing electron

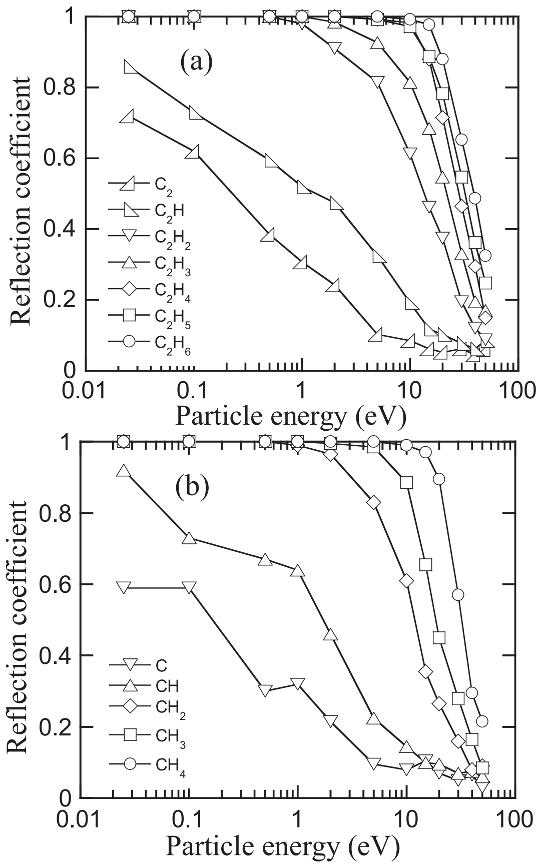

Fig. 5 Reflection coefficient for (a) C_2H_y ($y = 0 - 6$) and (b) CH_y ($y = 0 - 4$) on a hydrogenated and amorphized carbon surface [3].

temperature. In this study, the electron and ion temperatures are assumed to be equal. At the plasma temperature of 1, 5, 50, and 100 eV, the averages of the incident energy of C_2H^+ are 0.2, 1.5, 21.5, and 48.8 eV, respectively, and the reflection coefficients are 0.7, 0.5, 0.1 and 0.05, respectively. The plasma temperature dependence of the number of redeposited particles for molecular ions is due to the plasma temperature dependence of the reflection coefficient caused by sheath acceleration. In Fig. 5, with increasing hydrogen content in hydrocarbon molecules, i.e., x of CH_x and C_2H_x, the reflection coefficients increase because of weaker attraction interactions with surface carbon atoms. At the incident energy of up to 50 eV, the reflection coefficients of carbon, C_2H, and CH are smaller than those of other species. As a result, carbon, C_2H, and CH ions are the main redeposited species at temperatures ranging from 1 to 100 eV.

For C_2H^+ ions in the injection of C_2H_2, the sticking coefficients at 1 and 5 eV are 0.3 and 0.5, respectively, and the number of redeposited particles at 1 and 5 eV are 31 and 552, respectively. The ratio of the number of redeposited particles and the sticking coefficient is 103.3 at 1 eV and 1104 at 5 eV. These results indicate that the number of particles impinging on the divertor surface is greater at 5 eV than at 1 eV. The mechanisms causing the particles (neutral or ionized) to move to the divertor surface include the Lorentz force, friction force, and sheath potential. In this simulation, because the magnetic field strength and the plasma density are constant, the Lorentz and friction forces are also constant, and thus the mechanism of acceleration by the sheath potential is related to the number of impinging particles. The sheath force accelerates plasma ions located near the divertor surface, $z \leq 1$ mm, which corresponds to the sheath potential width. For plasma temperatures lower than 5 eV, the number of loss events of hydrocarbon molecules (ionization and dissociation processes) rapidly increases with plasma temperature. For example, the rate coefficients of $e^- + C_2H_2 \rightarrow C_2H + H$ at 1 and 5 eV are 0.75×10^{-10} and 0.26×10^{-8} cm^{-3}/s, respectively. For the injection of C_2H_2 molecule, the numbers of C_2H ion in the region of $z \leq 1$ mm is 112 at 1 eV and 1233 at 5 eV. Rapid increase in the number of redeposited particles at low plasma temperatures (≤ 5 eV) results from the increase in the number of break-up products in the sheath potential region. At low temperatures, this dependence holds true for the injection of C_2H_4 and C_2H_6.

4. Summary

In this study, hydrocarbon molecule transport in the modeled tokamak edge plasma region was studied by Monte Carlo simulation. Hydrocarbons in the ethane family were injected into the edge plasma and the local redeposited species on the divertor plate were examined. The number of redeposited particles increases with plasma temperature because of the increase in the impinging particle energy. This increase in energy is caused by acceleration by the sheath potential. The main redeposited species, C_2H and CH, were determined by the value of the reflection coefficient; hydrocarbon molecules with low hydrogen content have a low reflection coefficient because of weak attraction interactions with carbon atoms on the surface. For low plasma temperatures (≤ 5 eV), the number of redeposited particles suddenly increases with plasma temperature. This result is caused by a rapid increase in the number of hydrocarbon break-up products in the sheath potential region. The rate coefficients for loss events of hydrocarbon molecules with temperatures less than 5 eV play a crucial role in determining the density distribution of hydrocarbon molecular ions near the divertor plate ($z \leq 1$ mm).

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