A Kinetic Code System to Study Impurity Deposition and Fuel Retention in Gaps Between Divertor Tiles

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Received 31 March 2011, revised 23 November 2011, accepted 28 November 2011
Published online 04 May 2012

Key words Monte Carlo methods, particle-in-cell method, divertor, graphite.

For the purpose of investigating impurity deposition and fuel retention in gaps between divertor tiles, we combine a three-dimensional Monte Carlo impurity transport code ITCD with a Particle-In-Cell Monte Carlo collision code plus a plasma-surface interaction (PSI) code. The simulation results show that a potential hill formed near the entrance of the gap can prevent the ionized eroded carbon species from entering the gap. It is found that carbon sources for the co-deposition in gaps are mainly located at the plasma-closest edges of the gap, and this finding indicates that special measures associated with the engineering issues should be taken to minimize fuel retention in gaps. The smaller scale of carbon sources inside the gap and the existence of the potential hill near the entrance of the gap are the reasons why the eroded carbon species spatial density is lower inside the gap than outside the gap. Through the study on several scenarios with different substrate and plasma temperatures, the simulation with the combined code can deepen the understanding of fuel retention in the codeposited layers in gaps.

1 Introduction

The vertical targets of the divertor in the first phase of ITER operation will be made from carbon fibre composite (CFC) due to its good thermal shock resistance and tolerance to off-normal events, and they will be specially designed to be castellated structures for the purpose of maintaining the thermo-mechanical stability [1]. However, plasma facing components (PFCs) with castellated structures are exposed to a severe radiation environment with high power and particle fluxes, which lead to the erosion of carbon-based materials served as carbon sources for co-deposition with hydrogen isotopes. The deposition of the eroded carbon species can give rise to the build-up of tritium-rich carbon layers via co-deposition. Recently, the experiments performed in TEXTOR have evidently shown carbon accumulation and fuel retention in gaps with castellated structures [2-6]. Due to the shortage of effective cleaning techniques [7-11], continuous accumulation can lead to noticeable fuel retention in gaps. Some simulation works have been made to study plasma characteristics [12-13] and impurity transport and deposition [14-16] in gaps in present-day fusion devices.

A good knowledge of the locations of carbon sources and their corresponding contributions to the co-deposition is crucial for adopting effective measures to reduce the erosion of carbon-based materials and minimize fuel retention in gaps. This necessitates the development of computer simulation to make a detailed analysis of carbon sources and fuel retention in gaps. In this study, the simulation of impurity deposition and fuel retention in the poloidal gaps between divertor tiles has been performed using a kinetic code system, which consists of a two-dimension-in-space and three-dimension-in-velocity (2d3v) Particle-In-Cell Monte Carlo collision (PIC-MCC) code, a plasma-surface interaction (PSI) code, and a three-dimensional (3D) Monte Carlo (MC) impurity transport code ITCD [17]. The 2d3v PIC-MCC model [18] is similar to the 1d3v PIC-MCC model developed in our previous works [19-20] except being extended spatially to two dimensions. Applying the 2d3v PIC-MCC model to study plasma characteristics around the tile gap, we can provide the detailed information such as particle flux through the study on several scenarios with different substrate and plasma temperatures, the simulation with the combined code can deepen the understanding of fuel retention in the codeposited layers in gaps.

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and ion energy flux density as input parameters for the PSI model to evaluate erosion rate of carbon-based material [21]; then, the resulting erosion rate can be used as input parameters for the ITCD code to simulate impurity transport and deposition. Additionally, the studies on the influence of carbon substrate and plasma temperatures on the fuel inventory should provide useful information for understanding the characteristics of fuel retention in gaps.

2 Simulation models

In this study, we apply a kinetic code system to investigate impurity deposition and fuel retention in the poloidal gaps between divertor tiles. The kinetic code system consists of three sub-models: (i) 2d3v PIC-MMC model for studying the divertor edge plasma, (ii) plasma-surface interaction model for calculating erosion rate of carbon-based materials, and (iii) carbon and hydrocarbon impurity transport code ITCD. Figure 1 illustrates the schematic of the simulation domain and geometry of the poloidal gap. The simulation domain outside the gap is filled with the plasma with electron and ion temperature \( T_e = T_i \), and plasma density \( n_e = 1 \times 10^{19} \text{m}^{-3} \); no existence of the plasma initially inside the gap is assumed. The magnetic field lines are oblique to the wall surface of divertor tile, making an inclination angle of \( \alpha = 5^\circ \) with the wall surface. In the simulations, we set plasma temperature \( T_e = 20 \text{eV} \), carbon substrate temperature 600 K and magnetic field strength \( B = 2.5 \text{T} \) unless stated otherwise. These simulation parameters are similar to those in the outer divertor region of Chinese tokamak devices, HL-2A and EAST. The main purpose of this study is to report a basic physical process commonly existing in the edge plasma in tokamak devices. The plasma side and the plane of the gap bottom serve as the upper and bottom boundaries, respectively. The upper boundary is treated as an ideal plasma source. Periodic boundary conditions are applied in the y and z directions, and the z direction not shown in Fig. 1 is perpendicular to x-y plane.

![Fig. 1 The schematic of the simulation domain and geometry of the poloidal gap.](image)

The wall surface of divertor tile is set at the floating potential \( V_f = -3kT_e \) while the plasma side is set at the potential \( V_p = 0 \). In 2d3v PIC-MCC model, the Poisson’s equation is solved using multi-grid method. The collision processes for electrons and ions are handled by the Monte Carlo collision technique, and the collision reactions are summarized in Ref. [20]. The detailed information about PIC-MCC and PSI models can be found in the works [18-21]. The information flow among three sub-models is described as follows: the plasma species are driven in space by the electric and magnetic fields in 2d3v PIC-MCC model, and when they reach divertor target plate the detailed data such as particle flux and ion energy flux density are employed as input parameters for PSI model to evaluate the erosion rate of carbon-based materials; and then, the erosion rate can be used as input parameters for ITCD code to calculate the amount of eroded carbon species; finally, these eroded carbon species are tracked in ITCD model. In the PSI model, the physical sputtering and chemical erosion due to the bombardment of background hydrogen plasma are taken into account. The calculation of the physical sputtering yield of carbon atoms is based on the empirical formulae of Ref. [22]. The chemical erosion yield for carbon-based materials by hydrogen fluxes bombardment is calculated using the semi-empirical formulae [23]. It is
assumed that $CH_4$ molecules are generated by chemical erosion process and released into the plasma [15-16, 24-25]. In ITCD model, the tracked carbon species include hydrocarbon ions and neutrals, and ionized and atomic carbon particles.

The physical process of impurity transport in ITCD code [17] is described as follows: All eroded carbon species are released randomly from the bombarded points of the wall surface into the simulation domain. As a result of the eroded carbon species colliding with the plasma electrons and ions, many neutral and ionized fragments (i.e. carbon and hydrocarbons) are produced through chains of successive reactions. The collision probability of the eroded carbon species and its reactive fragments with background plasma is determined by plasma temperature and density [26]. The reactive rate coefficients involved here for carbon and hydrocarbons are taken from Ref. [27-28]. We also take into account the elastic collisions of carbon and hydrocarbons with the neutral hydrogen atoms by the hard sphere collision model, and the scattering angle and the energy loss factor are calculated according to Ref. [26]. All reactive fragments are tracked until they stick to the wall surface or leave the simulation volume. Neutral particles move along straight lines until they experience collisions. Charged particles gyrate due to Lorentz force in the magnetic field and undergo the friction, the thermal gradient force and cross-field diffusion [29]. Before an ionized particle comes to the wall surface, it must pass through a sheath region and is accelerated by the sheath field, and the sheath potential and electric field are calculated by the 2d3v PIC-MCC simulation code. When a particle comes to the wall surface, whether it sticks or reflects is determined by its reflection coefficient, which is different for different species and incident energies. These reflection coefficients have been calculated with different H/C ratios using the MolDyn and HCParcas molecular dynamics codes [30-32], and the reflection coefficients taken from the MolDyn code have been applied in our simulation (the H/C ratio and impact angle used in MolDyn code are 0.4 and 45°, respectively). The hydrogen inventory in gaps is estimated based on the formulae (3) of Ref. [33].

3 Results and discussion

3.1 Potential hill

Figure 2 shows the electric potential distribution around the entrance of poloidal gap. Here we can see that a so-called potential hill is formed near the entrance of the gap. This potential hill is formed due to different degree of magnetization of ions and electrons as discussed by R. Dejarnac et al [12-13].

This results in the charge separation and further producing a net positive charge region near the entrance of the gap. As can be seen from Fig. 2, the potential hill is positive and therefore repels the charged eroded carbon species from entering the gap. As a result, the number of the deposited eroded carbon species in the gap will reduce correspondingly. The quantification of the deposition rates of the ionized eroded carbon species in the gap is presented in Table 1(a). We perform the simulations to calculate the deposition rates of the ionized eroded carbon species for two cases: without and with potential hill. In the case without potential hill, the deposition rate of the ionized eroded carbon species is $3.40 \times 10^{17} m^{-2} \cdot s^{-1}$, however, the amount of the deposition rate decreases to $2.87 \times 10^{17} m^{-2} \cdot s^{-1}$ for the case with potential hill. Fig. 3 displays the deposition profile of the
ionized eroded carbon species along the gap for the cases with and without potential hill. It can be seen that the deposition rates for the case without potential hill are greater than that for the case with potential hill. Through the comparison of these two kinds of circumstances, we can see that the existence of the potential hill can reduce the amount of the ionized eroded carbon species in the gap and further hydrogen inventory in the codeposited layers. As shown in Fig. 2, the maximum of potential value is located at the centre of gap entrance. However, the potential value reduces gradually away from this centre. The potential values next to the sides of the gap are lower than that outside the gap, and at these regions the potential can’t prevent the charged eroded carbon species from entering the gap. This is the reason why the difference between the deposition rates for the cases with and without potential hill is not very pronounced.

Fig. 2 Deposition profile of ionized eroded carbon species along the gap for the cases with and without potential hill. The inset graph is the way of reading the distances.

3.2 Particle sources

Figure 4(a) presents the spatial distribution of the eroded carbon species density in the simulation domain. As can be seen, the eroded carbon species density can reach a value of about $5 \times 10^{17} m^{-3}$ next to the top surface of divertor tile, and the eroded carbon species density decreases gradually moving far away from the top surface. Figure 4(b) displays the eroded carbon species density spatial distribution in the poloidal gap. Take into account that the Larmor radii of plasma ions are comparable to the width of the gap and the tile walls will prevent them from coming into the gap, and hence, the erosion regions in the gap are located at the plasma-closest edges of the gap [17]. This makes clear the reason why the maximum of the eroded carbon species spatial density is located at the plasma-closest edges of the gap as shown in Fig. 4(b). In addition, it is very obvious that the eroded carbon species spatial density inside the gap is lower than that outside the gap. Inasmuch as the erosion area is much smaller inside the gap compared with the case outside the gap, the amount of the eroded carbon species which is proportional to the erosion area is smaller inside the gap. Further, the potential hill can prevent the ionized eroded carbon species outside the gap from entering the gap as mentioned above. Therefore, these reasons lead to the lower eroded carbon species spatial density inside the gap. A zoom-in of Fig. 4(a) labelled as Fig. 4(c) shows that the eroded carbon species density above the edge of side 4 is larger than that above the edge of side 1 due to the different erosion rates at the edges of these surfaces as shown in Fig. 5.

The plasma-wetted regions outside and inside the gap are acting as carbon sources, which are of vital importance to the study of fuel retention due to the co-deposition in gaps. Fig. 5 shows erosion rates for each side of the tiles. The corner of each tile serves as its position origin. The erosion characteristics around corner regions are different from that on top surfaces. This is mainly due to the existence of the potential hill near the entrance of the gap. The energies, fluxes and angles of incident particles in the corner regions vary greatly with the location due to the impact of the potential hill [18], which leads to different erosion rates at different locations as shown in Fig. 5. The results are illustrated in the inset graph of Fig. 5 which shows the erosion rates for side 2 and side 3 more clearly. As shown in the inset graph, the erosion rate for side 3 is slightly greater than that for side 2 when the erosion depth is over 0.2 mm. The works given by J. Roth et al showed that the chemical erosion
yield reduces when the incident particle flux is over a magnitude of about \(10^{22} \text{atoms} \cdot \text{m}^{-2} \cdot \text{s}^{-1}\) [23]. The larger ion flux \((10^{23} \text{atoms} \cdot \text{m}^{-2} \cdot \text{s}^{-1})\) for plasma-wetted side leads to a lower chemical erosion yield in our simulation [18]. As a result, the difference in the erosion rates between side 2 and side 3 is small. In addition, the erosion depth for side 3 is larger than that for side 2. To investigate the contribution of carbon sources with different erosion rates to the deposition of carbon species, we carry out more detailed analysis of the deposited carbon species in the gap stemming from which region: outside or inside the gap. The corresponding results are summarize in Table 1(b).

Table 1 (a) The deposition rates of the ionized eroded carbon species in the poloidal gap for two cases: without and with potential hill. (b) the deposition ratios of the eroded carbon species from outside and inside the gap and the corresponding hydrogen retention rates.

<table>
<thead>
<tr>
<th>(a)</th>
<th>The case without potential hill ((\times 10^{17} \text{m}^{-2} \cdot \text{s}^{-1}))</th>
<th>The case with potential hill ((\times 10^{17} \text{m}^{-2} \cdot \text{s}^{-1}))</th>
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<td>3.40</td>
<td>2.87</td>
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<th>(b) Particle sources</th>
<th>From outside the gap</th>
<th>From inside the gap</th>
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<tbody>
<tr>
<td>Deposition ratio of the eroded carbon species (%)</td>
<td>11</td>
<td>89</td>
</tr>
<tr>
<td>Hydrogen retention rates ((\times 10^{-6} \text{g cdot m}^{-2} \cdot \text{s}^{-1}))</td>
<td>0.13</td>
<td>1.12</td>
</tr>
</tbody>
</table>

The deposition ratio of the eroded carbon species is defined as the number of deposited carbon species from outside or inside the gap divided by the total number of the deposited carbon species in the gap. The deposition...
ratio of the eroded carbon species from outside the gap is 11%, while the deposition ratio of the eroded carbon species from inside the gap can reach up to 89%. The corresponding hydrogen retention rates for two cases are $0.13 \times 10^{-6} \text{g} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ and $1.12 \times 10^{-6} \text{g} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$, respectively. The implication of these results is essential for the engineering issues: the deposited carbon species in the gap are mainly originating from the plasma-closest edges of the gap, and accordingly, special measures should be taken in the process of engineering design to control the erosion of carbon-based material at this region, and then minimize the fuel inventory in the gap.

3.3 Hydrogen retention
In view of the importance of fuel retention in the fusion devices, we undertake further study on the characteristics of fuel retention under several scenarios. We investigate the variations of the fuel inventory by varying carbon substrate and plasma temperatures in the following subsections.

3.3.1 The influence of the substrate temperature
The amount of fuel retained in codeposits is fairly sensitive to the substrate temperature [34-36], which necessitates the performance of computer simulation to estimate the fuel inventory at different substrate temperatures. Profile of the hydrogen retention rate as a function of carbon substrate temperature is indicated in Fig. 6. It is shown that the hydrogen retention rate decreases with the increase in the carbon substrate temperature. The hydrogen retention rates do not show a significant difference when the substrate temperature is below 500 K. The curve of hydrogen retention rate drops dramatically in the substrate temperature range from 500 to 600 K. Above 600 K the trend of the curve becomes gentle by degrees with increasing the substrate temperature. At the substrate temperature of 300 K, the hydrogen retention rate is $3.46 \times 10^{-6} \text{g} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ shown in Fig. 6. In the cases of the substrate temperature 600 K and 900 K, the hydrogen retention rates reduce by a factor of three and eight, respectively, comparing with the case of the substrate temperature 300 K. The retention rates depend on the product of amount of deposited carbon species and hydrogen content. With increasing the surface temperature, the chemical erosion yield will increase slightly in our simulation, but the hydrogen content reduces. Therefore, the variation of the retention rates is the result of changing surface temperature in Fig. 6. Since the majority of carbon deposition occurs at the corners of the gap and these regions anyhow will be heated by the plasma to large surface temperatures, the level of fuel retention in gaps will be lower than expected. Also, it probably will be beneficial to the reduction of fuel retention in the deeper regions of gaps by increasing the substrate temperature in an appropriate range.
3.3.2 The influence of the plasma temperature

Inasmuch as most of the current diverter experiments show that the plasma temperature at the inner divertor region is different from that at the outer divertor region [7,37], it is necessary to check whether the plasma temperature has a strong impact on the hydrogen retention rate. The simulation results in Fig. 7 demonstrate the change in hydrogen retention rate with variation of the plasma temperature. It can be seen that hydrogen retention rate increases monotonically in the whole plasma temperature range shown in Fig. 7. The background plasma temperature has a significant bearing on the erosion of carbon-based material since which directly determines the incident energies of the plasma ions striking on the divertor tiles where the intense plasma surface interactions take place. At the plasma temperature of 5 eV, the erosion yield of carbon-based material is small, especially for physical sputtering yield; fewer energetic ions even though accelerated by the sheath field carry the kinetic energy over the threshold energy for physical sputtering, below which no physical sputtering occurs, and consequently, the erosion of carbon-based material at 5 eV is mainly due to the chemical erosion for which no threshold energy exists. With increasing the plasma temperature, the physical sputtering comes into play apart from the chemical erosion; meanwhile hydrogen plasma fluxes rise accordingly, which result in the increase of the amount of the eroded carbon species. Additionally, as the plasma temperature increases, the reactions between background plasma and eroded carbon species will intensify. This leads to increasing the number of carbon and hydrocarbons \( CH_y \) \((y < 4)\), which have lower reflection coefficients [30-31] and are apt to deposit in gaps. As a result, these reasons lead to the increase of hydrogen retention via co-deposition. As shown in Fig. 7, when the plasma temperature rises to 25 eV, the hydrogen retention rate increases to a value of \( 1.77 \times 10^{-6} \text{g} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \) and is five times higher than that at 5 eV.

In this work, the variations of the studied parameters are restricted to the poloidal gaps based on available computational capacity. However, the experiments have shown that the toroidal gaps contained comparable amount of carbon to that in the poloidal gaps [6]. Therefore, to estimate fuel retention in the entire gaps we assume the same deposition rates of carbon species in the poloidal and toroidal gaps. For typical ITER divertor, the dimensions of the tile are \( 19.5 \times 30 \text{mm}^2 \) and the surface area wetted by the plasma is \( 3.5 \text{m}^2 \) [38]. The total number of the gaps wetted by the plasma can be estimated to be of the order of 11500. When the plasma temperature rises from 5 to 25 eV, the corresponding hydrogen retention rates are in the range from \( 5.38 \times 10^{-6} \text{g} \cdot \text{s}^{-1} \) to \( 3.07 \times 10^{-5} \text{g} \times \text{s}^{-1} \) in the overall gaps. Applying this result to tritium, we obtain that the number of the discharges with a pulse length of 400 s would be of the order of magnitude of \( 10^4 \sim 10^5 \) before tritium retention in gaps reaches the safety limit of 700 g. Due to limited computational time, the studied parameters are restricted to several typical scenarios. Seeing that strong variation of plasma parameters (density and temperature) occurs along divertor plates, the calculated number of the discharges is a rough estimation.

4 Conclusions

In this work, we apply a kinetic code system consisting of (i) 2d3v PIC-MMC model, (ii) PSI model, and (iii) ITCD code to evaluate impurity deposition and fuel retention in gaps. We find that a potential hill formed near the entrance of the gap can prevent the ionized eroded carbon species from entering the gap. The smaller scale of carbon sources inside the gap and the existence of the potential hill near the entrance of the gap result in the
lower spatial density of eroded carbon species inside the gap. The majority of the deposited carbon species in the poloidal gap are derived from the plasma-closest edges of the gap. This result would be significant for the engineering design to reduce fuel retention.

By taking the erosion of realistic castellated surfaces (top and side surfaces of the tile) into account, the kinetic code system can provide quantitative analysis of fuel retention in gaps. We also find that the hydrogen retention rate reduces by a factor of eight when the substrate temperature increases from 300 to 900 K. In addition, the simulation results show that a low plasma temperature can lead to a visibly reduced hydrogen inventory. As a rough estimation, for the studied plasma temperatures, we estimate that the number of the discharges would be of the order of magnitude of $10^4 \sim 10^5$ before tritium retention in gaps reaches the safety limit.

Acknowledgements This work was supported by National Basic Research Program of China under grant No: 2008CB717801 and National Magnetic Confinement Fusion Science Program No: 2009GB106002. Authors would like to express their appreciation to F. Wang for his assistance in computation.

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