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Multiscale modelling of sheath physics in edge transport codes

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Abstract:

Power exhaust of fusion devices is determined by the interaction between the plasma and the wall of tokamaks. The way how fuel ions are reflected has a strong influence on the plasma temperature close to the surface. We investigate with the Soledge2D-EIRENE code different elements like sheath physics and surface roughness that have an effect on those interactions. We show that including realistic ion incidence angles based on 1D PIC sheath simulations provides a less efficient power exhaust than the original model where the ion cyclotron motion was not taken into account. The importance of the reflection database is also investigated considering two values of the Surface Binding Energy (SBE). This leads to consequent differences in the regions where the impact energy of deuterium ions is the smallest. Finally surface roughness is shown to have a positive effect on power exhaust.

1 Introduction

The extraction of power is a crucial issue for the operation of next step fusion devices. In particular, in ITER divertor, power flux can approach the material operation limit. In order to evaluate the divertor plasma conditions in ITER, modelling is required as no clearly identified scaling exist from present machines [1]. Simulations of the plasma edge transport are generally performed with a fluid code for the plasma and a kinetic Monte Carlo code for the neutrals. In the present work, we will rely on the Soledge2D-EIRENE code [2]. Plasma-surface interactions have a strong impact on the plasma parameters close to the surface. For instance, the particle reflection is influenced by the impact angle and energy of fuel ions hitting the surface as displayed in Figure 1(a). The way how the reflected atom is emitted will then have an effect on the plasma parameters in the vicinity of the surface as the power extraction is modified. Different elements have an effect on the impact angle. Here we will focus on the deflection by the magnetized sheath and on the surface roughness.

The effect of surface roughness on atomic processes has been investigated in previous works. Most of them however focus on the erosion and deposition processes where experimental evidence exists. A strong increase of deposition in the case of a rough surface compared to a smooth one has for example been observed in TEXTOR with the use of dedicated markers [3]. A modification of the TRIM.SP code [4] has also been performed to take into account the modification of the angle of incidence due to roughness measured by scanning tunneling microscopy [5]. Concerning the reflection, the effect of surface roughness has been investigated by modelling [6]. Computer simulations of the magnetic sheath with PIC codes [8, 9] have shown that the fuel ions arrive with grazing incidence ($\sim 10 - 20^\circ$ depending on the plasma parameters) on the surface. This is in agreement with predictions that can be made from a recent fluid model [10]. This tends to enhance the effect of surface roughness on surface processes as shown in [11, 12]. Finally concerning the influence of the energy reflection database, we can cite the comparison of plasma parameters between a carbon and a tungsten wall that have different reflection properties and that has been carried out in [13].

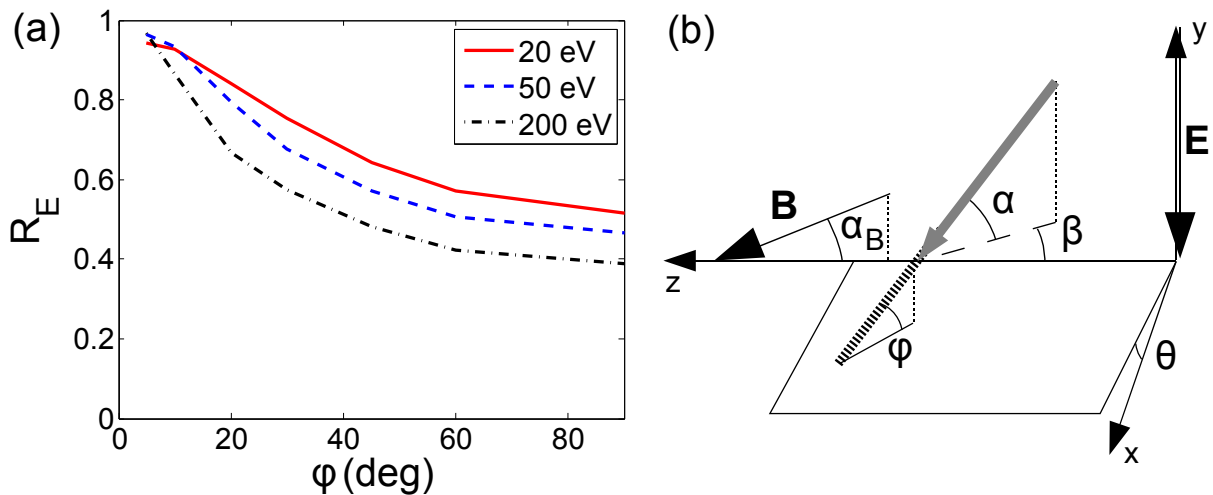


FIG. 1: (a) Dependence of the energy reflection coefficient R_E on the incidence angle for 3 different impact energies. (b) Schematic view of the different angles involved.

2 Model

The angles and geometry of the plasma-surface interaction are shown in Figure 1(b). Displayed are: α_B the angle between the flat surface and the magnetic field, α the impact and β the twisting angles of the impinging particle on the flat surface, φ the incidence angle of the particle on the rough surface and θ the angle between the rough surface and the flat surface.

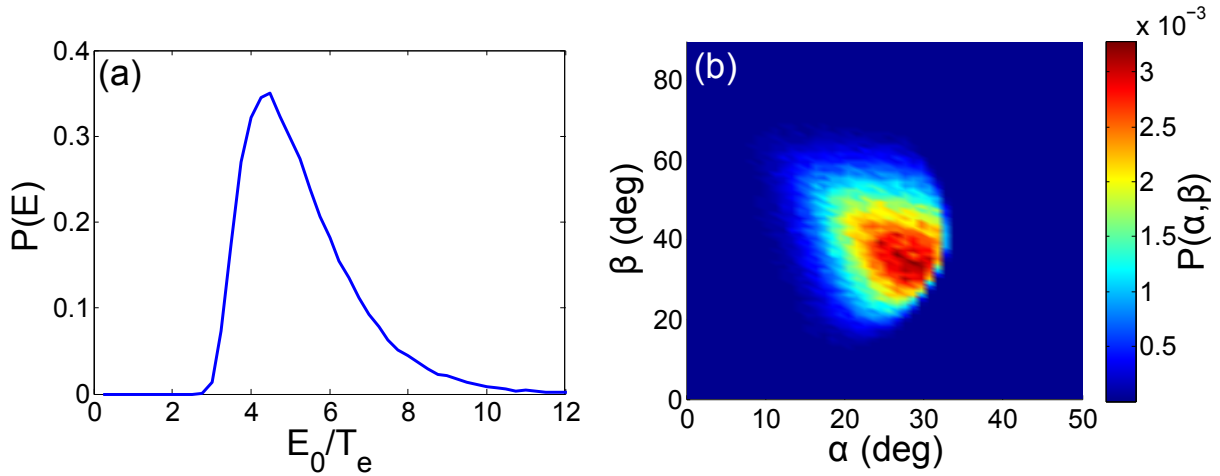


FIG. 2: Impact energy (a) and angular (b) distributions in the case $\alpha_B = 3^\circ$, $\zeta = 30^\circ$ and $\tau = 1$ that is relevant for divertor parameters.

2.1 Sheath simulations

The magnetized sheath affects the reflection of fuel ions by determining its impact angle and energy. Whereas the energy increase inside the sheath is generally well taken into account, only simple models for the impact angle of particles exist in the edge codes. In order to obtain more reliable impact angle data, self-consistent simulations of the magnetized sheath are carried out with a 1D PIC code [7]. The code injects the particles (ions and electrons) at the sheath entrance and simulates their trajectories in the electric field that is computed by Poisson's equation. Three parameters are required to span all the different cases and could be found by normalisation of the set of equation: α_B , $\zeta = r_L/\lambda_D$ the magnetisation parameter that is the ratio between the Larmor radius ($r_L = c_e/\omega_{ci}$, ω_{ci} being the ion cyclotron frequency and $c_e = \sqrt{T_e/m_i}$ the cold ion sound speed) and the debye length λ_D and, finally, $\tau = T_i/T_e$ the ionic to electronic temperature ratio.

Simulations including average values of the impact angle $\langle \alpha \rangle$ and impact energy $\langle E \rangle$ have been carried out in [14]. Those values have been provided in EIRENE as a function of the plasma parameters computed by Soledge2D. Here we will investigate the full distribution of impact angles and energy using the joint Probability Density Function (PDF) of α , β and E knowing the three parameters required in the PIC simulations $P(\alpha, \beta, E|\zeta, \alpha_B, \tau)$. Such a distribution is given as an example in Figure 2. The distribution in energy is peaked around $E_0/T_e = 5$, which is in agreement with the usual formula for the impact angle at the surface ($2T_i + 3T_e$). The angular distribution is quite concentrated with most of the impacts in the region $20^\circ < \alpha < 30^\circ$ and $25^\circ < \beta < 45^\circ$.

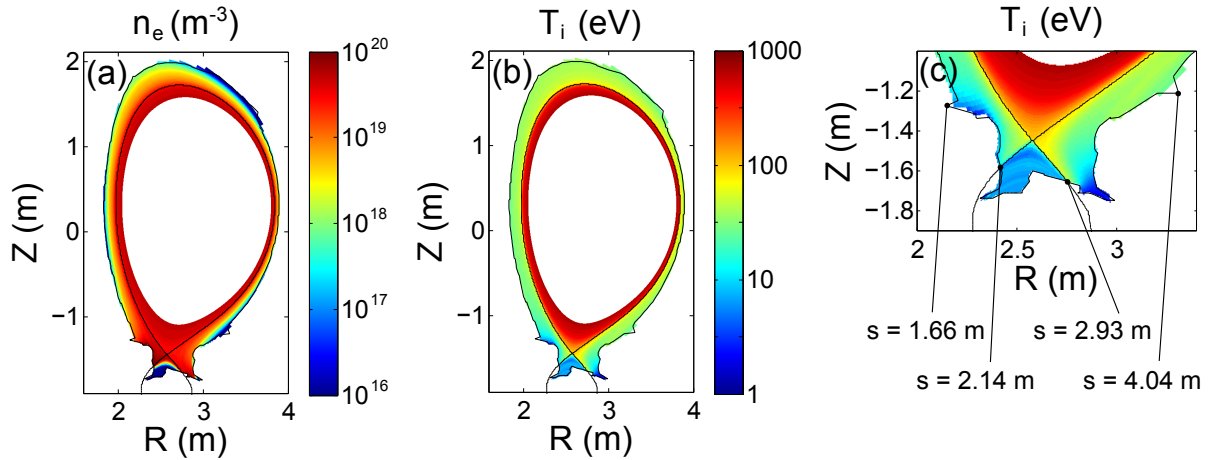


FIG. 3: Electron density (a) and ion temperature (b) obtained with Soledge2D-EIRENE for the JET configuration considered. (c) Zoom on the divertor for the ion temperature with four wall coordinate s positions.

2.2 Surface roughness

In order to assess the potential effect of surface roughness on the plasma temperature at the border of the plasma, a simple model has been implemented in EIRENE. The local orientation θ (see Figure 1(b)) is modified for each particle impacting on the wall. This provides a new angle with respect to the impinging ion velocity but this also modifies the ejection angle of the released particle. The rotation of the wall element is determined according to a Gaussian distribution of θ and limited from -90° to 90° . Several consistency tests are carried out to ensure that the impinging ion hitting the surface arrives with $\varphi > 0$ and that the ejected particle velocity is oriented towards the plasma and not inside the wall.

3 Results

Simulations are performed in a case based on the shot #83559 in JET that has been carried out with the ITER-Like Wall (ILW). The electron density and ion temperature are displayed in Figure 3. The case is partially detached: very low ion temperature is achieved at the inner strike point while the leg of the outer strike point is still visible in Figure 3(b). A zoom on T_i in the divertor is performed in Figure 3(c). The value of the wall coordinate s is displayed at different locations and will be used when presenting the results. They will concentrate on the tungsten divertor (W) even if, except for the reflection dependence on the surface binding energy that applies only to tungsten (the first wall is in beryllium (Be)), effects are considered everywhere in the chamber.

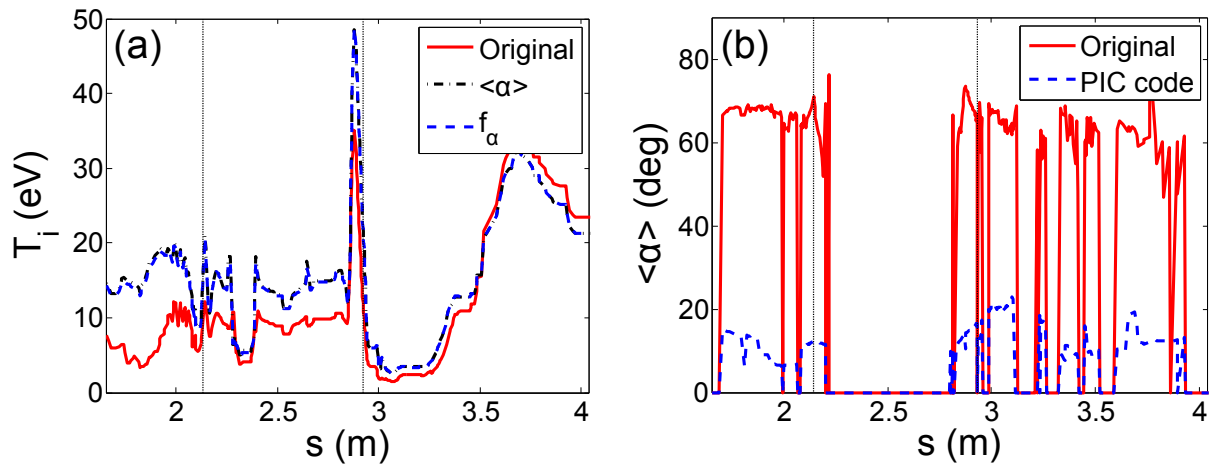


FIG. 4: (a) Ion temperature in the vicinity of the surface for the original model (plain, red), the average impact angle and energy (dash-dot, black) and the full distribution (dash, blue) based on PIC simulations. (b) Average impact angle for the original model (plain, red) and PIC simulations (dash, blue). Dotted vertical lines correspond to strike point locations.

3.1 Sheath treatment

Results of the simulations with the different sheath treatments are displayed in Figure 4(a). The ion temperature is larger when the data from the PIC simulations are used than with the original model expect around the baffle at $s > 3.5$ m. The original model is based on Maxwellian distributions at the sheath entrance, for which the sheath acceleration is added in the direction perpendicular to the surface. This leads to some very large angles (60-70°) as shown in Figure 4(b). The value calculated with the PIC code are much smaller leading to a stronger energy reflection of deuterium and, as a consequence, to an increase of T_i close to the surface. The results obtained with the full distribution of impact energies and angles exhibit almost no differences with the average values. This can be explained partially by the relatively peaked energy and angular distributions of the ions when they hit the surface (see Figure 2).

3.2 Surface binding energy

Reflection database used in EIRENE are calculated by the SDTrimSP code [15]. An important input parameters is the Surface Binding Energy (SBE), which has a strong effect on reflection but also on other processes like sputtering. Originally, $SBE = 1$ eV has been used and is far from the estimated value for W ($SBE = 8.68$ eV). In order to evaluate its importance on the plasma parameters close to the wall, comparison with an intermediate value of SBE (5.53 eV) has been carried out. The energy reflection coefficient for both values of SBE is provided in Figure 5(a) at $\alpha = 20^\circ$, which is relevant with the impact angle obtained by the PIC code (see e.g. Figure 4(b)). Above ~ 300 eV, no difference is observed. Under this value, however, the discrepancy can be very large,

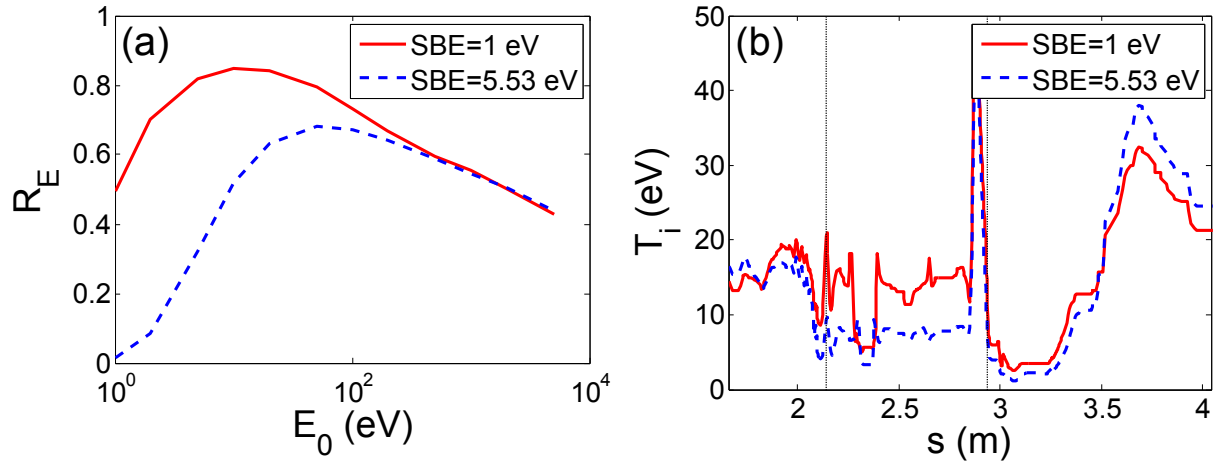


FIG. 5: (a) Energy reflection coefficient at $\alpha = 20^\circ$ for $SBE=1$ eV (plain, red) and $SBE=5.53$ eV (dash, blue). (b) Ion temperature in the vicinity of the surface with reflection database calculated with $SBE=1$ eV (plain, red) and $SBE=5.53$ eV (dash, blue). Dotted vertical lines correspond to strike point locations.

especially at very low impact energy. The results of the comparison between the two values of SBE are displayed in Figure 5(b) for the case where the impact angles from PIC simulations have been used. A reduction of a factor 2 in the private region and close to the inner strike point is observable. In this region the impact energy implies a large difference between the reflection for the two values of SBE. A smaller difference is observable in other places where the impact energy is larger. Like in the case where the different models for the sheath were compared, the opposite behaviour is seen close to the baffle. Note that contrarily to the effects studied here, the modification applies only to the W part of the wall.

3.3 Surface roughness

The last simulation has been conducted with a model surface roughness described by a gaussian distribution whose root mean square is $\theta_{rms} = 10^\circ$. Results are shown in Figure 6 compared with the flat surface case. The impact angles from PIC simulations have been used. A strong reduction of the ion temperature is again observed close to the inner strike point parallel to an increase on the baffle. Two effects can be identified. First, in a general way, the average impact angle is increased by the roughness. In the case of very grazing incidence (take for example $\alpha = 10^\circ$), it is unlikely that this angle can be diminished - the angle of the surface θ needing to be larger than -10° - but it can be strongly increased as no limitation when θ is positive exists. Larger impact angle means reduced energy reflection and thus a reduced ion temperature. Second, the angle of ejection of the particles is reduced by the roughness (a cosine ejection angular distribution has been considered). Considering the geometry close to the inner strike point (Figure 3(c)), a larger number of ejected particles will return to the surface than at the baffle

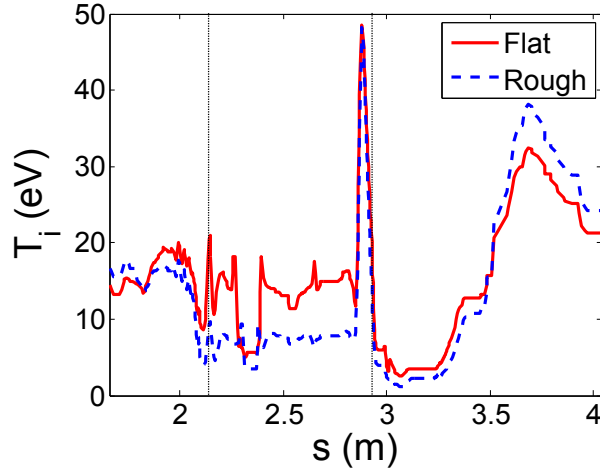


FIG. 6: Ion temperature in the vicinity of the surface with a flat surface (plain, red) and a rough surface with $\theta_{rms} = 10^\circ$ (dash, blue). Dotted vertical lines correspond to strike point locations.

and evacuate in an easier manner the energy. The strong variation of ion temperature observed in Figure 6 has probably to be attributed to both effects.

4 Conclusions

The effect of plasma-surface interactions on the ion temperature in the vicinity of the surface has been investigated. Calculations based on a half-detached case in JET have been performed. Modelling of the average impact values obtained with a 1D PIC code have shown an increase of the temperature due to the more grazing incidence as when the sheath was taken into account in a simplified manner. The implementation of the full distribution does not change the results in a significantly. The reflection database has been shown to affect the temperature in an even stronger manner than when the PIC simulations angles were used. In the JET case investigated, the deuterium ion impact the surface with an energy lower than 100 eV in most of the divertor region. At those energies a discrepancy exists between the different value of the SBE. Finally the influence of the surface roughness has been studies by the use of a simple model. It increases the local incidence angle and induces a reduction of the ion temperature in the vicinity of the surface.

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