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Atomic processes leading to asymmetric divertor detachment in KSTAR L-mode plasmas

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Abstract

The experimentally observed in/out detachment asymmetry in KSTAR L-mode plasmas with deuterium (D) fueling and carbon walls has been investigated with the SOLPS-ITER code to understand its mechanism and identify important atomic processes in the divertor region. The simulations show that the geometrical combination of a vertical, inner target with short poloidal connection from X-point to target and a much longer outer divertor leg on an inclined target lead to neutral accumulation towards the outer target, driving outer target detachment at lower upstream density than is required for the inner target. This is consistent with available Langmuir probe measurements at both target plates, although the inner target profile is poorly resolved in these plasmas and further experiments with corroborating diagnostics are required to confirm this finding. The pressure and power loss factors defined in the two-point model [1-4] of the divertor scrape-off layer (SOL) and the sources contributing to the loss factors are calculated through post-processing of the SOLPS-ITER results. The momentum losses are mainly driven by plasma-neutral interaction and the power losses by plasma-neutral interaction and carbon radiation. The presence of carbon impurities in the simulation enhances pressure and power dissipation compared to the pure D case. Carbon radiation is a strong power loss channel which cools the plasma, but its effect on the pressure balance is indirect. Reduction of the electron temperature indirectly increases the momentum loss by decreasing the static pressure and increasing the volumetric reaction rates which are responsible for the loss of momentum. As a result, the addition of carbon saturates the momentum and power losses in the flux tube at lower upstream densities, reducing the rollover threshold of upstream density. The relative strengths of the various mechanisms contributing to momentum and power loss depends on the radial distance of the SOL flux tubes from the separatrix (near/far SOL) and the target (inner/outer target). This is related to the strong D_2 molecule accumulation near the outer strike point, which makes the deuterium gas density at the outer target 2-10 times higher than that at the inner target. A large portion of the recycled neutral particles from both targets reach and accumulate in the outer SOL, which is attributed in strong part to the target inclination and gap structure between the central and outboard divertors and hence to the impact of geometry. The accumulated neutrals enhance the reactions involving D_2 which cause momentum and power loss.

1. Introduction

Heat fluxes deposited on the tokamak divertor plates need to be controlled for the sustainable operation of future fusion reactors, including ITER and DEMO. If solid material targets are to be used, the detached divertor regime is considered to be the main mechanism for heat flux control, but the detailed mechanisms involved in the process remain arguable. As the upstream electron density is increased by gas fueling, the pressure and power losses along the flux tubes in the scrape-off layer (SOL) are accompanied by rollover of the target parallel ion flux, which leads to the detached regime. According to previous work (see e.g. [5,6]), volumetric recombination and impurity

radiation are important actors in the achievement of strong detachment, but there is still much discussion about the extent to which plasma-neutral friction can lead to detachment by providing a significant fraction of momentum loss [1]. In principle, the detachment characteristics are device-dependent because the pressure and power losses which are governed, for example, by volumetric reactions and flux expansion, are also influenced by the physical divertor geometry and wall material [7]. Density ramp experiments in ASDEX-U and JET showed that the inner (i.e., high-field side (HFS)) target rolls over at a lower line-averaged electron density, \bar{n}_e , than the outer (i.e., low-field side (LFS)) target [8-10]. In contrast, the opposite detachment behavior was reported in TCV for configurations with very much longer poloidal lengths of the divertor leg in comparison with the inner [11,12]. The causes of asymmetry in divertor detachment have been attributed to the divertor (magnetic) geometry and drift motion of charged particles. However, it is still often the case that the detailed experimental observations cannot be quantitatively matched by plasma boundary simulation codes.

This paper presents analysis using the SOLPS-ITER code of a core plasma density scan experiment in KSTAR using D_2 fueling. We attempt to understand the process of divertor detachment and its asymmetric behavior by examining the momentum and power balances with a detailed source term decomposition as in Kotov [2] and Moulton [4]. The asymmetric detachment behavior of KSTAR, where the experimental ion flux rolls over at a lower \bar{n}_e at the outer target than at the inner, is consistent with the simulations and can be understood in terms of the impact of the neutral deuterium distribution on the pressure and power balance. In turn, it appears that a major contributing factor to this distribution can be attributed to the physical divertor geometry in KSTAR. Drift flows, which are not yet activated in our SOLPS-ITER simulations, may well change the picture, but since drifts cannot be switched off in experiment and the observed asymmetries and detachment behaviour are similar to that seen by the code, it seems reasonable to conclude that geometry effects are important.

2. KSTAR L-mode divertor detachment experiments

A series of L-mode deuterium density scan experiments have been conducted in KSTAR single lower diverted discharges. The main plasma density was feedback-controlled by adjusting the deuterium gas puffing rate. In these plasmas the toroidal magnetic field $B_T = 1.8$ T, was in the forward (clockwise) direction putting the ion $B \times \nabla B$ direction downwards into the lower divertor. The plasma current was $I_p = 0.5$ MA ($q_{95} = 5$) with 0.7 MW of neutral beam heating. As shown in Fig. 1(a), among the three divertor targets in the lower divertor, the strike points were placed on the inboard and central divertor regions. The density was scanned over a total of 4 discharges from $\bar{n}_e = 1.5 \times 10^{19} \text{ m}^{-3}$ to $3.0 \times 10^{19} \text{ m}^{-3}$ and kept constant during each of the discharges. The line averaged density was measured with a horizontal interferometer chord passing through the mid-plane.

Outer divertor strike point sweeping, performed twice in each discharge, was performed across the fixed, embedded divertor target Langmuir probes (LP) to obtain profiles of parallel ion saturation current (particle flux density, Γ_{\parallel}). As shown in Figure 2, which compiles the time dependences of \bar{n}_{e} and a pair of LPs on each target in the strike point vicinity, there was no significant impact (<10% variation) of the sweeping on the main plasma density. This outer target sweep leads to a smaller amplitude vertical motion of the inner strike point, providing a more restricted HFS sweep. As consequence of this insufficient sweep amplitude and the fixed spatial locations of the probes, the inboard target particle flux profiles are unfortunately incomplete. Reconstructed Γ_{\parallel} profiles derived from the sweeps are compiled in Fig. 1(b), showing how particle flux rollover starts first at the LFS ($\bar{n}_e = 2.0$ -2.5×10¹⁹ m⁻³), followed by the HFS at the higher upstream density ($\bar{n}_e = 2.5 - 3.0 \times 10^{19} \text{ m}^{-3}$). Unfortunately, although several other diagnostics of importance to a simulation study of the kind reported here are installed on KSTAR, during these particular experiments, many were unavailable due to hardware faults (e.g. edge Thomson scattering, total radiation bolometry) or did not produce data of sufficient quality to be of use (divertor target infra -red camera, main SOL fast reciprocating Langmuir probe). We note that the missing portion of the inner target flux density profiles means that the observation of inner target detachment beginning at lower upstream density at the outer target should be taken with some caution and needs to be confirmed in further studies with improved diagnostic coverage.

While a detachment asymmetry in which the outer target detaches at lower \bar{n}_e than the inner target is in

contrast to the general finding in other tokamaks, it was similarly observed on TCV in single null lower discharges [11,12], though in the latter case with reversed B_T . Both KSTAR and TCV are full carbon wall devices and for the experiments in [11,12] TCV employed a similar divertor geometry to that of the KSTAR discharges reported here; namely the inner strike point on a vertical target with short poloidal distance to the X-point and the outer strike point on a horizontal plate with much longer poloidal distance from X-point to target. However, the TCV configuration had 10-20 times higher outer divertor poloidal leg length than the inner, whilst this ratio is only 2-3 on KSTAR. The principal origin of the unusual asymmetric detachment observed in KSTAR is not therefore considered to be the relative difference of divertor leg length but seems to be related to other features of the divertor geometry.

3. Setup of SOLPS-ITER simulations

The SOLPS-ITER code suite [13,14] (version 3.0.6), which includes the multi-fluid plasma solver B2.5 and Monte Carlo neutral tracer EIRENE, has been utilized to model the KSTAR response to these L-mode density ramp experiments. In fact, the observation of earlier LFS than HFS detachment was seen first in code density scans before it was found experimentally. Scans of the outer mid-plane (OMP) separatrix electron density $n_{e,sep}$ were conducted stepwise from $n_{e,sep} = 0.5 \times 10^{19} \text{ m}^{-3}$ to $3.7 \times 10^{19} \text{ m}^{-3}$ with feedback-controlled D₂ gas puffing rates. The simulation grid shown in Fig. 3(a) was built on magnetic geometry obtained by an EFIT reconstruction for discharge #19077 at time = 5.0 s, corresponding to the middle of the flattop. A given SOL ring on the numerical grid is defined as a collection of grid cells in the SOL region with the same radial index. To distinguish the SOL plasma behavior with respect to distance from the separatrix, three representative SOL rings (1st SOL ring (near-SOL), 9th SOL ring (mid-SOL), and 17th SOL ring (far-SOL) – see Fig. 3(b)) were selected among the 18 rings constituting the fluid plasma grid. Detailed particle, momentum, and power balance analyses were conducted along these three rings and will be discussed below.

The simulations were performed with and without carbon as a sputtered impurity. The decay lengths of the ion density and the ion and electron temperatures at the outer grid boundary were set to 3 cm. The power injected into the numerical grid of 0.5 MW was assumed to be evenly distributed to the electrons and ions. Due to the absence of the bolometer data, an assumption is required regarding the power to inject into the simulation grid: among the total NBI heating of 0.7 MW, 30% was assumed to be radiated, constant with density. In common with most plasma boundary code studies, cross-field transport of particles and heat is assumed to be diffusive with anomalous diffusion coefficients of $D_{\perp} = 0.5 \text{ m}^2 \text{s}^{-1}$ for particles and $\chi_e(\chi_i) = 1.0 \text{ m}^2 \text{s}^{-1}$ for heat. The reactions used in EIRENE are listed in Table 1. The pumping surface is set to be the highlighted region in figure 3(a) for numerical simplicity, instead of extending the grid to the end of the port similar to the real geometry on KSTAR [15]. The simulation pumping surface is toroidally extended and the total area is 5.5 m^2 with absorption probability set to be 0.2. For the simulation sets including carbon, the chemical sputtering yield is set to 1% and the physical sputtering calculated using the TRIM database [16]. Deuterium ions are assumed to be completely recycled from material surfaces, and cross-field drifts are not activated, though it is clear that they would be expected to impact the degree of in-out target asymmetry [17]. Such simulations are much more challenging and the aim of this paper is to examine whether or not the observed detachment asymmetry can be explained by other mechanisms, notably divertor geometry.

4. Asymmetric divertor detachment

Simulations with $n_{e,sep} \ge 2.8 \times 10^{19} \text{ m}^{-3}$ were not included here because of the unrealistically low electron temperature (< 25 eV) at the OMP separatrix, which are considered to be achievable only in the numerical simulation. The highest density case considered in the simulations was $n_{e,sep} = 2.77 \times 10^{19} \text{ m}^{-3}$, corresponding to $0.4 n_{GW}$, where n_{GW} is the Greenwald limit [18] of the target discharge (KSTAR shot #19077): $I_p = 0.5 \text{ MA}, a = 0.5 \text{ m}$).

Figure 4(a) shows the predicted total parallel particle flux Φ_{\parallel} as a function of $n_{e,sep}$ for the inner and outer targets and the two different cases of pure D and D+C. Here Φ_{\parallel} is the integral of Γ_{\parallel} over the parallel cell area at each target across the entire profile. Figure 4(b) gives the simulated target parallel particle flux (Γ_{\parallel}) for the 3 SOL rings specified earlier and can be compared qualitatively with the analogous experimental result in Fig. 1(b). For the D+C case, rollover in Φ_{\parallel} occurs at $n_{e,sep} \ge 1.10 \times 10^{19} \text{ m}^{-3}$ at the outer target and $n_{e,sep} \ge 1.74 \times 10^{19} \text{ m}^{-3}$ at the inner target. The trend is similar to the experimental observations described in Section 2. Target particle fluxes in the outer divertor SOL rings, $\Gamma_{\parallel}^{\text{ot}}$, rollover simultaneously at all locations at $n_{e,sep} = 1.10 \times 10^{19} \text{ m}^{-3}$. However, on the inboard side, the mid and far-SOL ring fluxes, $\Gamma_{\parallel}^{\text{it}}$ begin to decrease at much higher densities ($n_{e,sep} = 1.73 \times 10^{19} \text{ m}^{-3}$ and $n_{e,sep} = 2.35 \times 10^{19} \text{ m}^{-3}$, respectively), implying partial detachment only. Without carbon, the outer and inner target flux roll-over occurs at slightly higher densities of $n_{e,sep} = 1.40 \times 10^{19} \text{ m}^{-3}$ and $n_{e,sep} = 2.02 \times 10^{19} \text{ m}^{-3}$, respectively.

After the rollover, the predicted outer target Φ_{\parallel} reduces to 5.37×10^{21} s⁻¹ for the D+C case and 9.89×10^{21} s⁻¹ for pure D case at the highest simulated upstream densities. Compared to the peak value, the outer target Φ_{\parallel} is reduced to 45% and 70% for the D+C case and the pure D case, respectively. Particle flux removal is thus lower for the pure D case and may be attributed at least partly to the absence of carbon radiation [19]. The peak value of Φ_{\parallel} at both of the inner and outer targets in the D+C case is 20% smaller than the case without carbon. Furthermore, the value of Φ_{\parallel} in the case of D+C is lower than in the case of pure D after rollover. According to the two-point modelling formatting (2PMF) equations [1-4] (see [1] Section 4 for detailed explanation of each of the terms and variables in the equations), this means that carbon either reduces upstream total pressure $p_{tot,u}$ or enhances momentum loss in the flux tube:

$$T_{\text{et}}^{2\text{PMF}} = \left[\frac{8m_{i}}{e\gamma_{t}^{2}}\right] \left[\frac{q_{\parallel u}^{2}}{p_{\text{tot,u}}^{2}}\right] \left[\frac{(1-f_{\text{power}})^{2}}{(1-f_{\text{mom}})^{2}}\right] \left[\left(\frac{R_{u}}{R_{t}}\right)^{2}\right] \left[\frac{(1+T_{\text{it}}/T_{\text{et}})}{2}\right] \left[\frac{(1+M_{t}^{2})^{2}}{4M_{t}^{2}}\right]$$
(1)
$$\Gamma_{\text{e}\parallel t}^{2\text{PMF}} = \left[\frac{\gamma_{t}}{8m_{t}}\right] \left[\frac{p_{\text{tot,u}}^{2}}{q_{t}}\right] \left[\frac{(1-f_{\text{mom}})^{2}}{(1-f_{t})}\right] \left[\left(\frac{R_{t}}{R_{t}}\right)\right] \left[\frac{2}{(1+T_{t}/T_{t})}\right] \left[\frac{4M_{t}^{2}}{(1+T_{t}/T_{t})}\right]$$
(2)

$$\sum_{i=1}^{2PMF} = \left[\frac{r_t}{8m_i}\right] \left[\frac{r_{tot,u}}{q_{\parallel u}}\right] \left[\frac{(1-f_{power})}{(1-f_{power})}\right] \left[\left(\frac{n_t}{R_u}\right)\right] \left[\frac{2}{(1+T_{it}/T_{et})}\right] \left[\frac{m_t}{(1+M_t^2)^2}\right]$$
(2)

$$f_{T_{\text{et}}}^{\text{vol-loss}} = \left[\frac{(1-f_{\text{power}})^2}{(1-f_{\text{mom}})^2}\right]$$
(3)

$$f_{\Gamma_{\parallel \text{et}}}^{\text{vol-loss}} = \left[\frac{(1 - f_{\text{mom}})^2}{(1 - f_{\text{power}})}\right]$$
(4)

$$\Gamma_{e\parallel t}^{\text{basic 2PM}} = \left[\frac{\gamma_t}{8m_i}\right] \left[\frac{p_{\text{tot,u}}^2}{q_{\parallel u}}\right]$$
(5)

Equations (3) and (4) represent the volumetric loss terms responsible for the determination of target electron temperature and the target flux, respectively. Since $R_u/R_t \approx T_{it}/T_{et} \approx M_t \approx 1$ in this simulation, the correction of the basic two-point model prediction of T_{et} and $\Gamma_{e\parallel t}$ is mainly governed by the volumetric loss terms. The momentum and power loss factors f_{mom} and f_{power} are defined as the loss fractions of the total pressure p and internal energy flux q_{\parallel} along the flux tube from upstream (u) to the target (t):

$$(1 - f_{\text{mom}})p_{u} = p_{t},$$

$$f_{\text{mom}} = -\int_{t}^{u} S_{\text{mom}} ds_{\parallel}/p_{u},$$

$$(1 - f_{\text{power}})q_{\parallel u}A_{\parallel u} = q_{\parallel t}A_{\parallel t},$$

$$f_{\text{power}} = -\int_{t}^{u} S_{\text{IE}} dV/q_{\parallel u}A_{\parallel u}$$
(6)

where A_{\parallel} , s_{\parallel} , dV, S_{mom} , and S_{IE} are the surface area of the mesh cell normal to the parallel direction, the length parallel to the magnetic field from the target to the upstream, mesh cell volume $(ds_{\parallel}A_{\parallel})$, the source of the total pressure, and the source of the internal energy, respectively [2,20]. For the calculation of f_{mom} and f_{power} , the upstream point is chosen here as the X-point for both the inner and outer SOL.

Figure 5(a)-(b) show Φ_{\parallel} calculated using the basic 2PM and 2PMF approaches. The former predicts that Φ_{\parallel} is nearly identical regardless of the presence of carbon except for $n_{e,sep} > 2.0 \times 10^{19} \text{ m}^{-3}$. The difference in Φ_{\parallel} between 2PMF and the basic 2PM is caused by the volumetric loss term (Eq. (4)). This is because the terms in Eq. (1) excluding the terms in Eq. (4) and (5) are almost unity for the KSTAR lower single null case. Since the reduced Φ_{\parallel} from the beginning of the rollover due to the inclusion of carbon is only reproduced in the 2PMF prediction, the term in Eq. (4) is responsible for it. This means that carbon not only enhances power loss through the radiation, but also the momentum loss necessary for roll-over of the target flux through reduction of T_e consistent with the 2PMF. Carbon radiation itself is not accounted for in the pressure balance, but it indirectly enhances momentum loss by cooling the background plasma. Figure 5(c) shows the volumetric loss term for the target particle flux. The roll-over (and reduction) of $f_{\Gamma_{\parallel et}}^{\text{vol-loss}}$ for all SOL rings means that the momentum loss is enhanced relative to the power loss and this leads to the roll-over of the target flux. Except for the 17th SOL ring of both targets, the carbon indirectly enhances momentum loss; the roll-over of $f_{\Gamma_{\parallel et}}^{\text{vol-loss}}$ occurs at the lower $n_{e,\text{sep}}$. When carbon is added to the simulation, $f_{\Gamma_{\parallel et}}^{vol-loss}$ shifts to the lower densities, however the shape of the plots in Fig. 5(c),(d) remains similar. Therefore, the slope of the curves in Fig. 4(a) does not change much when carbon is included. As the rollover of $f_{\Gamma_{\parallel et}}^{vol-loss}$ begins, $f_{T_{et}}^{vol-loss}$ starts to increase and suppresses further reduction of the target T_{et} (Fig. 5(e),(f)). Since volumetric recombination is only significant when the plasma approaches $T_e \sim 1 \text{ eV}$, the predicted trends in the simulation prevent the code from accessing recombining condition, which may assist roll-over of the target flux [5,6,19].

5. Results and Discussion

5.1 Pressure and power losses

To characterize the processes leading to detachment predicted by the SOLPS-ITER simulations, the momentum and power loss mechanisms are examined in more detail in this section. Although the 2PMF volumetric loss terms in Eq. (3) and (4) describe the overall effect of the volumetric reactions on the target plasma parameters through the loss of the total pressure and the power along a given flux tube, it is not straightforward to decompose them into contributions from each of the reactions in Table 1 because the 2PMF equation is in multiplicative rather than additive form. We thus proceed in the analysis presented here to decompose of f_{mom} and f_{power} into the various source terms, i.e., the sources S_{mom} and S_{IE} including perpendicular transport, parallel viscosity, and neutral related reactions from EIRENE as given in Table 1 [2]. These quantities are then integrated along the flux tubes from the target to the user-defined upstream point (the X-point in this case).

Beginning first with the overall loss factors, as shown in Fig. 6(a)-(c), f_{mom} increases with $n_{e,sep}$. One immediate observation is that plasma pressure balance is not satisfied for all SOL rings, even under low recycling conditions ($n_{e,sep} < 1.10 \times 10^{19} \text{ m}^{-3}$), especially in the outer target far-SOL rings ($f_{mom} \sim 0.5$ -0.7). Momentum loss is indirectly enhanced by including carbon in the simulation, but the saturated level of f_{mom} is similar to the case without carbon. The slight f_{mom} rollover at high density in the near-SOL occurs as a result of the loss of momentum beyond the X-point in the detached regime (see Section 5.2, Fig. 7). Figure 8(a)-(c) shows the decomposition of the outer SOL f_{mom} for the pure D case. As a consequence of perpendicular diffusion, almost 30% of the upstream total pressure is lost in the near SOL under low recycling conditions (low upstream density). With increasing $n_{e,sep}$ and the onset of detachment, the diffusive loss fraction decreases. At this point, volumetric reactions are the dominant momentum loss. Parallel viscosity provides a slight momentum gain, mainly due to the Bohm sheath boundary condition [21], which forces the parallel velocity near the target to match or exceed the sound speed. The momentum gain is most significant (20% of the upstream total pressure) in the mid-SOL ring, low recycling condition where the perpendicular transport and the volumetric reactions are negligible.

Atom-plasma (Electron Impact Ionization, EI and Charge Exchange, CX) and molecule-plasma reactions (D₂pl.) given in Table 1 are the dominant momentum losses/gains determining f_{mom} under high recycling and detached conditions. As $n_{e,sep}$ increases, losses due to the (EI, CX) first increase, followed by (D₂-pl.). At higher density ($n_{e,sep} > 2.0 \times 10^{19} \text{ m}^{-3}$), their contribution roll over, due to the definition of the X-point as the "upstream" location. They still contribute actively to the momentum loss near the outer mid-plane beyond the X-point (see Section 5.2, Fig. 7).

In the outer target far SOL, the atom-plasma processes actually result in a momentum gain; this is a result of i) momentum transfer from the energetic deuterium atoms (D) to the cold deuterium ions (D^+) through charge-exchange and ii) asymmetry of the distribution functions between deuterium atoms and ions caused by neutrals recycled mainly from the outboard divertor target (see neutral particle trajectories shown in Fig. 9). Including carbon in the simulation, the overall trend of the momentum loss contribution is unchanged (Fig. 8(d)-(f)). The carbon radiation itself does not, of course, contribute to the momentum balance in the simulation. However, the plasma is cooled more quickly relative to the case without carbon due to the increased radiation, enhancing the pressure losses by promoting volumetric reactions which are sensitive to the electron temperature.

Regarding f_{power} there is a slight rollover in the near SOL of both inner and outer targets as $n_{e,sep}$ is increased (Fig. 6(d)-(f)). This is due to the onset of significant power dissipation beyond the X-point (see Section 5.2, Fig. 7) with increasing $n_{e,sep}$. Therefore, when the upstream reference point is selected as a higher upstream location, such as the outer/inner mid-plane, the rollover of f_{power} and f_{mom} does not occur. Including carbon increases f_{power} , with saturation at lower $n_{e,sep}$ than when it is absent (pure D). In common with f_{mom} , the saturated level of f_{power} is similar for both pure D and D+C simulations.

Figure 10(a)-(c) presents the decomposition of the contributions to f_{power} in the outer divertor SOL for the case without carbon. Among the volumetric reactions, EI is always the dominant power loss channel except for the outer divertor far SOL ring, where molecule-ion reactions are the biggest contributor. Charge-exchange between the D atoms and ions transfers power from D to D⁺, resulting in an average plasma power gain rather than loss. This is consistent to the abovementioned momentum transfer from the energetic deuterium to the cold deuterium.

The dissociation and ionization of D₂ molecules also lead to power losses. However, the sum of both contributions are predicted to amount to 10%–30% of the total power loss only, which depends on $n_{e,sep}$ and the particular SOL ring. Under low recycling conditions, perpendicular transport from the near SOL to the private flux regions (PFR) is responsible for most of the power loss (Fig. 10(a),(d),(g)). This loss channel is replaced by volumetric losses by the beginning of the rollover. The inner far SOL ring (Fig. 10(i)) exhibits a low power loss fraction for all divertor regimes ($f_{power} = 0.2-0.6$). In contrast, f_{power} is already significant in the outer target far SOL ring (Fig. 10(c) and (f)) in the low recycling regime ($f_{power} \sim 1$), remaining high under high recycling and detached conditions.

Unlike in the other SOL regions studied, the main cause of power loss for the outer target far SOL ring (Fig. 10(c) and (f)) is molecule-related reactions: molecule-electron reactions in low recycling conditions and moleculeion reactions (including elastic and CX between D₂ and D⁺) after rollover. Here, the power loss due to the moleculeion reactions is compensated by the power gain due to CX between D and D⁺. The code finds that energetic D⁺ is first generated by CX between D and D⁺ followed by a loss of D⁺ energy via interactions between D₂ and D⁺.

The carbon radiation directly contributes to the power balance. Comparing figures 10(a)-(c) and (d)-(f), the power loss trends remain similar with an additional power loss due to the carbon. The radiation loss due to the presence of carbon monotonically increases with rising $n_{e,sep}$ (Fig. 11(e)). The main radiators are C³⁺ and C²⁺ with a smaller contribution from C⁺, consistent with observations in carbon wall devices such as DIII-D [22]. As the upstream density increases, the two-dimensional distribution of the carbon radiation source changes. At the lowest density (Fig. 11(a)), the radiation sources are localized at the outer target, moving upstream with increasing $n_{e,sep}$ to become more concentrated near the X-point when target plate detachment begins but still in the divertor SOL (Fig. 11(b)-(c)). When $n_{e,sep}$ increases further, the radiating zone extends into the core region around the X-point (Fig. 11(d)), corresponding to the penetration inside the separatrix of medium carbon charge states (e.g. C³⁺) which are powerful radiators in the VUV spectral region (X-point MARFE [23]). At this point, up to 25% of the total input power in the simulation domain is radiated in the near SOL and the X-point regions.

5.2 Distributions of volumetric reaction and neutral densities

The deuterium molecular and atomic distribution affect the strength of the volumetric reactions and plasma parameters such as T_{et} (see e.g. [3]). The target D₂ density n_{D2t} is a monotonically increasing function of $n_{e,sep}$ while the target D atom density, n_{Dt} rolls over right across the outer target but only slightly in the near SOL of the inboard target (Fig. 12). This can be explained by the variation of the volumetric reaction front position depicted in Fig. 7. The normalized positions of the ionization, molecule-plasma reaction, and carbon radiation fronts are defined here as

$$\langle s_{\parallel,\mathrm{EI}} \rangle = \frac{\int_{\mathrm{t}}^{\mathrm{u}} s_{\mathrm{EI}} s_{\parallel} ds_{\parallel}}{\int_{\mathrm{t}}^{\mathrm{u}} s_{\mathrm{EI}} ds_{\parallel}},\tag{7}$$

$$\langle s_{\parallel,\text{mol-pl}} \rangle = \frac{\int_{t}^{u} s_{\text{mol-pl}} s_{\parallel} ds_{\parallel}}{\int_{t}^{u} s_{\text{mol-pl}} ds_{\parallel}},\tag{8}$$

$$\langle s_{\parallel, \text{rad}, \text{C}} \rangle = \frac{\int_{\text{t}}^{\text{u}} s_{\text{rad}, \text{C}} s_{\parallel} ds_{\parallel}}{\int_{\text{t}}^{\text{u}} s_{\text{rad}, \text{C}} ds_{\parallel}},\tag{9}$$

where s_{\parallel} is the normalized parallel length from the target ($s_{\parallel} = 0$) to upstream ($s_{\parallel} = 1$) and S_{EI} , S_{mol-pl} , $S_{rad,C}$ are the number of electron impact ionization per mesh cell, the number of D₂ – plasma reaction per mesh cell and the power source per mesh cell caused by carbon radiation, respectively. In this section, upstream now refers to the OMP rather than the X-point since the fronts can be located beyond the X-point.

Under low recycling conditions ($n_{e,sep} < 1.10 \times 10^{19} \text{ m}^{-3}$ for the D+C case, before the rollover of outer target flux), the ionization front is located well below the X-point in the near- and mid-SOL at both inner and outer divertors. As $n_{e,sep}$ increases, the ionization fronts of the outer divertor SOL rings move from the outer target through the X-point to the OMP, while in the inboard divertor, the ionization front remains between the target and X-point in the inner SOL except for the highest density case. As the ionization front moves upstream, the neutral atoms originally localized at the target spread out upstream. In addition, when T_e near the target drops below 2 eV, D₂ is no longer dissociated, reducing the D source and triggering the rollover of n_{Dt} (see Fig. 13).

The molecule-plasma front is usually located further downstream than the ionization front, as expected. At the lowest $n_{e,sep}$, the relative location of the two fronts can be reversed and this happens for the outer mid- and far-SOL flux tubes (Fig. 7(b) and (c)). According to the neutral particle trajectories in the low recycling conditions (Fig. 9(a) and (b)), the molecules (green lines in Fig. 9) penetrate upstream through the gap between the plasma grid and the outboard divertor target. With the exception of the inner target far-SOL, the molecule-plasma front steadily moves upstream with increasing $n_{e,sep}$. As a result, molecules penetrate further upstream but n_{D2t} increases due to the longer molecule dissociation time near the target. The fronts in Eq. (7)-(9) of the inner target far-SOL are localized near the X-point. This is because the inner target far-SOL is immediately adjacent to the X-point due to the geometry (Fig. 3(a)), and most of the neutral particles are found at the near- and mid-SOL of the inner SOL.

Adding the carbon as an impurity to the simulation, $\langle s_{\parallel,EI} \rangle$ and $\langle s_{\parallel,mol-pl} \rangle$ are located further upstream; consistent with the momentum and power balance analysis, carbon cools the plasma, helping to shift the position of the reaction fronts upstream, given the very sensitive temperature dependence of the front location. The reaction fronts refer to the relative position where the reaction occurs most actively in each of the SOL rings. However, it does not indicate the absolute amount of the contribution to the power and momentum balance. As shown in the Fig. 7 and 11, $\langle s_{\parallel,rad,C} \rangle$ rises in the near-SOL of both targets. Parameter $\langle s_{\parallel,rad,C} \rangle$ is meaningful only in the near-SOL ring where dominant radiation occurs (Fig. 11).

As shown in Fig. 12, the target deuterium molecule density n_{D_2t} at the outer target is 2–10 times higher than that at the inner target, demonstrating a significant asymmetry. Figure 9 throws some light on this observation through 2D plots of the EIRENE kinetic neutral trajectories. Particles launched at the outer target (Fig. 9(b), (d)) mostly reside in the outer SOL regardless of the divertor condition. However, those originating at the inner target mainly penetrate the plasma and are confined by collisions in the outboard divertor SOL at low density (Fig. 9(a)). As the divertor regime changes to the high recycling and detached conditions (Fig. 9(c)), the majority of the neutrals still move to the SOL through the PFR but a significant fraction is trapped by collision in the inboard SOL. Globally, most neutrals recycled from the two targets access the gap between the outboard and central divertor targets leading to an accumulation of D_2 in the space below the divertor structure. A strong D_2 accumulation near the far-SOL ring of the outer target is attributed to the target inclination, which drives the neutrals outwards and to the effective Vshape between the central and outboard divertor target preventing neutral escape from the corner. Molecules penetrate further into the inboard divertor SOL, but reside primarily in the near-SOL or PFR of the inner target vicinity rather than the far SOL ring of the inner target, as shown in Fig. 13.

Following [1], a correlation analysis has been conducted between T_e , f_{mom} and n_{D_2t} . Since the 1st and 2nd SOL rings are dominated by the perpendicular transport, and the 10th to 18th rings have relatively small particle fluxes, they have been excluded from the analysis, which focuses only on rings 3-9. Simple linear regression results finds a strong correlation between n_{D_2t} and the target electron temperature: $T_{et} = 3.68 \times 10^{24} n_{D_2t}^{-1.28}$ with R-squared of 0.94 (Fig. 14(a)). Note that the values are taken at the last computational cell before the guard cells which the code uses for the purposes of imposing boundary conditions at the target sheaths. This has also been observed elsewhere in simulation studies and is discussed in detail in [1,3]. According to the momentum balance shown in Figure 8, the losses due to the molecule related volumetric reactions (D₂-pl.) increase monotonically as a function of $n_{e,sep}$, which is an increasing function of n_{D_2t} (Fig. 12). Therefore, the ion drag force induced by collisions with molecules is responsible for plasma cooling below 5 eV where the other loss mechanisms do not operate. The slope of the curve in Fig. 14(a) becomes steeper for $T_{\rm e} < 1 \, {\rm eV}$ where $n_{\rm Dt}$ decreases and $n_{\rm D_2t}$ increases as $T_{\rm et}$ decreases. Here, the molecule-plasma reactions dominate over all other reactions. The momentum loss factor similarly correlates strongly with T_{et} (Fig. 14(b)), as also seen in simulations of other devices such as C-Mod, AUG, JET [1,24] and also experimentally [25]. Note that the computation of upstream and downstream pressures used to obtain f_{mom} are performed using the real flow values calculated by the code (i.e. not imposing unity Mach number at the target $(M_t = 1)$ or $M_u = 0$ at the upstream location). As shown in Fig. 14 (c), the momentum loss factor due to the molecule-plasma reactions becomes the dominant loss mechanism for $T_{\rm e} < 1 - 2$ eV where molecular dissociation, no longer occurs. The total momentum loss and n_{D_2t} are also highly correlated (Fig. 14(d)). This can also be explained by the ion drag force due to the molecules.

The asymmetric T_{et} between inner and outer target from the aforementioned D₂ accumulation in the gap between the central and outboard divertors affects the spatial variation of the volumetric reactions: (i) inner/outer target and (ii) near/mid/far SOL. In the D₂-predominant SOL ring (i.e., the outboard divertor far-SOL), the pressure loss is mainly due to molecule–plasma reactions, and the power loss to molecule–ion reactions. In the other SOL rings, the dominant pressure loss originates from atom–plasma reactions (EI and CX), and the power loss predominantly due to EI. Although the strong correlation between the neutral particle distribution and the volumetric reactions (and T_e , especially near the target) that determine important momentum and power loss mechanisms and divertor regime are observed in the SOLPS-ITER study, the cause and effect, and in particular the influence of divertor geometry, cannot be unambiguously identified without further studies.

6. Conclusions and future work

The SOLPS-ITER plasma boundary code suite has been used to simulate an L-mode density scan in KSTAR carbon wall, single null lower deuterium, forward toroidal field discharges with an asymmetric divertor configuration in which the inner strike point is located on a vertical target with short poloidal length from X-point to target and the outer strike point is placed on the slanted, central divertor region (in between a horizontal and vertical target) with longer poloidal distance to the X-point. Experimentally, as the upstream density increases, particle flux rollover is first observed at the outer target, followed by the inner target at higher density. This is in contrast to the majority of observations on divertor tokamaks operating in forward field direction, where rollover/detachment is observed to occur first at the inboard target. The behaviour found in the simulations is qualitatively consistent with experiment and it is notable that the pure deuterium simulations described in this paper were actually performed before the experiment on KSTAR was run, thus constituting a prediction of the detachment asymmetry.

Detailed analysis of the simulation results, including decomposition of the various contributions to momentum and power losses in selected inner and outer divertor flux tubes, allows the following picture of the process to be established. A strong D₂ source near the outer target leads to: (i) an increase in n_{D_2t} , (ii) a decrease in T_{et} and $(1 - f_{mom})$, (iii) movement of the fronts of electron ionization and ion-molecule reactions from downstream to upstream and rollover of n_{Dt} , and (iv) cooling of the overall flux tube and further increase in momentum and power loss caused by the volumetric reactions. Carbon radiation promotes additional power losses, contributing to a favorable environment for other volumetric reactions (EI, CX, DS in Table 1) to occur at lower upstream electron density. However, the mechanism of momentum and power losses remains similar. Since n_{D_2t} at the outer target is 2–10 times larger than that of the inner target, earlier detachment is observed at the outer target in the simulations, in agreement with the experimental observations.

In these simulations, drifts and currents have not been activated in the SOLPS-ITER simulations because of the very challenging additional complexity. It is well known that drifts have a strong influence on power and particle sharing in the divertor in current devices [17, 26, 27] and the conclusions reached here based purely on the simulations are likely to be modified if drifts are switched on. Such simulations are planned, but the analysis presented here clearly shows that divertor geometry must have an impact on the observed detachment behaviour. To further clarify the geometrical effect on the asymmetrical distribution of the neutral particle, additional simulations with divertor geometry scans are also planned.

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Index	Related species	Reaction	Туре
1	Atom, plasma	$D + e \rightarrow D^+ + 2e$	EI
2		$D^+ + D \rightarrow D + D^+$	CX
3		$C + e \rightarrow C^+ + 2e$	EI
4		$D^+ + C \to C^+ + D$	CX
5	Molecule, plasma	$e + D_2 \rightarrow 2e + D_2^+$	EI
6		$e + D_2 \rightarrow e + D + D$	DS
7		$e + D_2 \rightarrow 2e + D + D^+$	DS
8		$D^+ + D_2 \rightarrow D^+ + D_2$	EL
9		$D^+ + D_2 \rightarrow D + D_2^+$	CX
10	Test ion, plasma	$e + D_2^+ \to e + D + D^+$	DS
11		$e + D_2^+ \rightarrow 2e + D^+ + D^+$	EI
12		$e + D_2^+ \rightarrow 2D$	DS
13	Plasmas	$C^+ + e \rightarrow C$	RC
14		$D^+ + e \rightarrow D$	RC

Table 1. Reactions used in the EIRENE code. The definitions are as follows. EI: electron-impact ionization, CX: charge exchange, DS: dissociation, EL: elastic collision, and RC: recombination.

FIGURE CAPTIONS

Figure 1. (a) Magnetic configuration of the described density scan experiment in KSTAR. The numbers on the plot indicate the channel number of the fixed divertor Langmuir probes. (b) Parallel-B particle flux profiles on the targets measured by Langmuir probes in four discharges (shot #19077, #19078, #19079, #19085) as a function of the distance from the strike point (+: SOL, -: private flux region) on each of the targets with different upstream averaged densities as specified in the legend. The numbers on the figure indicate \bar{n}_e in 10^{19} m⁻³.

Figure 2. Shot sequence of the density scan experiments. Line averaged electron density \bar{n}_{e} and parallel target particle flux measured by Langmuir probes (see figure 1(a) showing the location of the specified channel number as LP##) from top to bottom, respectively. The strike point sweeping was performed twice during each discharge. The numbers on the curves in each figure denote \bar{n}_{e} in 10^{19} m⁻³.

Figure 3. (a) SOLPS-ITER grid for the simulated KSTAR equilibrium. The locations of the gas puffing slot and pumping surface are specified. (b) SOL rings for pressure and power balance analysis: near-SOL ring (1st), mid-SOL ring (9th), and far-SOL ring (17th).

Figure 4. SOLPS-ITER predicted target fluxes. (a) Total parallel particle flux Φ_{\parallel} as a function of $n_{e,sep}$. The solid lines are the cases with carbon (D+C) and the dashed lines are the pure D cases. (b) Parallel particle flux density at the target Γ_{\parallel} as a function of $n_{e,sep}$ for the case with carbon (D+C) on the three flux tubes in Fig. 3(b) at both targets. Target flux profile for the low recycling ($n_{e,sep} = 0.5 \times 10^{19} \text{m}^{-3}$), high recycling ($n_{e,sep} = 1.1 \times 10^{19} \text{m}^{-3}$, where rollover of outer target starts) and detached ($n_{e,sep} = 2.75 \times 10^{19} \text{m}^{-3}$) conditions at (c) inner target and (d) outer target.

Figure 5. (a) and (b) Basic 2PM and 2PMF total target particle fluxes on the target for inner and outer targets,

respectively. (c)-(f) 2PMF volumetric loss terms from SOLPS modelling as a function of $n_{e,sep}$ on the three flux tubes in Fig. 3(b). (c) and (d) $f_{\Gamma_{\parallel}et}^{vol-loss}$ for inner and outer target, respectively. (e) and (f) $f_{T_e}^{vol-loss}$ for inner target and outer target, respectively. Solid and dashed lines represent the case with carbon (D+C) and pure D, respectively.

Figure 6. Top row: f_{mom} in Eq. (6) on the three flux tubes in Fig. 3(b). Lower row: f_{power} in Eq. (6) on the three flux tubes in Fig. 3(b). Solid and dashed lines represent the case with carbon (D+C) and pure D, respectively.

Figure 7. $\langle s_{\parallel,EI} \rangle$, $\langle s_{\parallel,mol-pl} \rangle$ and $\langle s_{\parallel,rad,C} \rangle$ defined in Eq. (7)-(9) along the three flux tubes in Fig. 3(b) as a function of $n_{e,sep}$. Solid and dashed lines represent the case with and without carbon respectively. (a)-(c) Outer SOL and (d)-(f) Inner SOL. The outer SOL ionization fronts move upstream of the X-point (horizontal dashed line) in high recycling and detached regime while the inner SOL ionization fronts are mostly located under the X-point.

Figure 8. Pressure loss along the three outer SOL flux tubes in Fig. 3(b) normalized to p_u as a function of $n_{e,sep}$. (a)-(c) represents the pure D case and (d)-(f) shows the case with carbon (D+C). The thick blue curve indicates f_{mom} in Eq. (6). EI and CX represent atom-plasma reactions in Table 1. D₂-pl. represents the molecule-plasma reactions in Table 1. The orange and red dotted curves are the pressure losses due to perpendicular transport and parallel viscosity, respectively.

Figure 9. EIRENE kinetic neutral trajectories for the case with carbon are shown for two density levels specified on each row. (a), (c) Test particles are launched from the inner target. (b), (d) Test particles are launched from the outer target.

Figure 10. Power loss along the three flux tubes in Fig. 3(b) normalized by $q_{\parallel}A_{\parallel}$ as a function of $n_{e,sep}$. The thick blue curve represents f_{power} in Eq. (6). EI and CX represent EI of D and CX between D and D⁺, respectively. (D₂, D⁺) represents CX and EL between D₂ and D⁺. (D₂, e) represents DS and EI of D₂ by interactions with electrons. The orange dotted curve is the power loss due to perpendicular transport. The gray line is the power loss due to the carbon radiation. (a)-(c) Outer SOL pure D, (d)-(f) Outer SOL with carbon (D+C), (g)-(i) Inner SOL with carbon (D+C).

Figure 11. (a)-(d) 2D distribution of the carbon radiation. (b) and (c) correspond to the case at Φ_{\parallel} rollover of the outer target and the inner target, respectively. (e) Total carbon radiation power as a function of $n_{e,sep}$.

Figure 12. Density of D (dashed) and D₂ (solid) at the (a) outer target and (b) inner target as a function of $n_{e,sep}$. The blue, orange, and yellow curves represent the 1st, 9th and 17th SOL rings, respectively.

Figure 13. Two-dimensional distributions of (a) D and (b) D₂ with $n_{e,sep} = 2.35 \times 10^{19} \text{ m}^{-3}$.

Figure 14. (a) Scatter plot of the target electron temperature as a function of the target deuterium molecule density. The solid line is a linear regression with $T_{\text{et}} = 3.68 \times 10^{24} n_{\text{D}_2\text{t}}^{-1.28}$ with R-squared of 0.94. (b) The remaining momentum fraction $(1 - f_{\text{mom}})$ at the target compared to the upstream as a function of the target electron temperature (c) The ratio of the momentum loss factor due to the molecule-plasma reaction to the total momentum loss factor $(f_{\text{mom}}^{\text{mol}-\text{pl}}/f_{\text{mom}})$ as a function of target electron temperature (d) $(1 - f_{\text{mom}})$ as a function of the target deuterium molecule density.



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