

# Using SOLPS to confirm the importance of total flux expansion in Super-X divertors

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**Abstract.** We show that a central characteristic of Super-X divertors, total flux expansion  $f_R$  (defined as the ratio of the elementary area normal to the magnetic field at the target to that at the X-point), significantly changes the characteristics of the target plasma for fixed upstream conditions. To isolate the effect of total flux expansion from other effects, we utilise SOLPS-5.0 simulations of an isolated slot divertor leg in a minimally complex, rectangular geometry. The grid is rotated outwards about a fixed X-point in order to perform a scan in which only the total flux expansion increases, by means of a decrease in the target magnetic field at higher major radius. We find that if the SOL remains in the attached, conduction-limited regime throughout the scan, the target electron density scales approximately as  $f_R^2$ , while the target electron temperature scales approximately as  $1/f_R^2$ , in good agreement with the modified two-point model presented in (Petrie T W *et al* 2013 *Nucl. Fusion* **53** 113024). If, however, the SOL transitions from the sheath-limited regime to the conduction-limited regime during the scan, the simulated scalings of target electron temperature and density are weaker than predicted by the modified two-point model. The upstream density for transition from sheath- to conduction-limited regimes is found to scale approximately with  $1/f_R$ , in agreement with the modified two-point model. Assessing upstream-density-driven detachment onset, we find that the target electron temperature at which target density rollover occurs ( $\sim 0.6$  eV) is independent of  $f_R$ . Given this, the modified two-point model predicts a halving of the upstream (and target) densities at which rollover occurs when  $f_R$  is doubled, in good agreement with the simulation results.

## 1. Introduction

The Super-X divertor has been proposed as a means to reduce the large plasma energy flux densities and physical sputtering at the targets of fusion reactors (Kotschenreuther *et al* 2010). There are two defining aspects of a Super-X divertor which distinguish it from a conventional divertor: (i) increased major radius at the target relative to the X-point (this leads to an increased total flux expansion from X-point to target, which in

turn leads to a reduced parallel energy flux density at the target<sup>‡</sup>); (ii) increased parallel and poloidal distances from X-point to target. In addition, the Super-X divertor of the forthcoming MAST-Upgrade machine (Fishpool *et al* 2013) will use a baffle around the divertor entrance to increase the neutral compression relative to conventional divertors.

In this contribution, we isolate and study the effect of increased total flux expansion. From conservation of magnetic flux we have that  $dA_{\parallel t}B_t = dA_{\parallel u}B_u$ , where  $dA_{\parallel}$  is the elementary area normal to the total magnetic field  $B$  and subscripts  $t$  and  $u$  denote target and X-point (‘u’ for ‘upstream’) quantities, respectively. We define the total flux expansion as  $f_R \equiv dA_{\parallel t}/dA_{\parallel u} = B_u/B_t \approx R_t/R_u$ , where  $R$  is the major radius. In the model used here, the ratio of poloidal and toroidal magnetic field components is kept constant (with both assumed to be inversely proportional to  $R$ ) so that the latter approximation is, in fact, exact.

Several authors have addressed the effect of total flux expansion on attached divertor conditions using variations of the two-point model (Petrie *et al* 2013, Kotschenreuther *et al* 2010, Stangeby *et al* 2000). Petrie *et al* (2013) predicted that in the attached, conduction-limited phase, the target electron density and temperature scale approximately with  $f_R^2$  and  $1/f_R^2$ , respectively. Lipschultz *et al* (2016), using a model based on energy balance, predicted that the upstream density required for detachment onset scales with  $1/f_R$ , while the upstream density required for the thermal front to reach the X-point is independent of  $f_R$  (i.e. the detachment ‘window’ increases with  $f_R$ , making detachment control easier). If shown to be true, such strong effects would greatly benefit the Super-X divertor over the conventional divertor, by decreasing the physical sputtering yield (for the same upstream collisionality), lowering the upstream collisionality at which detachment onset occurs, and making detachment easier to control. This could potentially bring closer the ultimate goal of a detached target plasma that is compatible with a steady-state, reactor-relevant, low-collisionality core plasma with self-sustained current drive.

In *realistic* geometries, however, experimental and modelling analyses are more mixed in their support of total flux expansion. (Havlíčková *et al* 2015) showed that, for the same upstream conditions, the MAST-Upgrade Super-X divertor leads to a higher density, lower temperature target plasma than a conventional divertor. That difference meant that the Super-X also detached at lower upstream density. (Umansky *et al* 2016), in contrast, reported that their UEDGE modelling of several different divertor configurations show little effect of the target major radius on the detachment input power threshold. (Theiler *et al* 2016) reported that, in TCV experiments, the line-averaged electron density at which the target ion flux rolls over is indistinguishable when the target major radius is increased by a factor 1.3. (Petrie *et al* 2013) showed that the target electron density and temperature depend only weakly on target major radius in DIII-D. The authors proposed that this was due to changes in the neutral pathways as

<sup>‡</sup> This also results in a reduced energy flux density *felt* by the target if, by decreasing the poloidal magnetic field at the target, the angle between the target plate and the total magnetic field is kept constant as the strike point major radius is increased.

the target was swept out; the higher target major radius configuration also had a more open divertor, potentially attenuating the effect of increased total flux expansion.

In all of these realistic geometry studies (both experimental and modelling), it is impossible to eliminate confounding variables when scanning the total flux expansion. These can include (but are not limited to) the neutral pathways, radial transport in the divertor, SOL width at the divertor entrance, pitch angle, impurity content, parallel and poloidal distances from X-point to target – all of which can change when the target major radius is moved in a real tokamak. The role of total flux expansion alone is therefore difficult to assess. On the other hand, two-point models like the one presented by (Petrie *et al* 2013) leave out physics which may, in reality, be important (e.g. neutral physics, radial transport, viscosity, unequal electron and ion temperatures, non-unity target Mach numbers and the transition from sheath- to conduction-limited regimes).

In this study, we attempt to bridge the gap between models with simplified geometry and simplified physics, and models (or experiments) with realistic geometry and realistic physics, by assessing a model with a simplified geometry and more realistic physics than accounted for by (Petrie *et al* 2013). This model utilises SOLPS-5.0 in an isolated, rectangular, slot divertor leg. By rotating the leg about the X-point, a scan is performed in which the only parameter that changes is the total flux expansion. The scalings of the target plasma in the face of the additional physics of SOLPS-5.0 are then compared to those of (Petrie *et al* 2013). Furthermore, we perform upstream density scans for the two extremes of our total flux expansion scan, in order to assess the effect of total flux expansion on the transition from sheath- to conduction-limited regimes and on detachment onset.

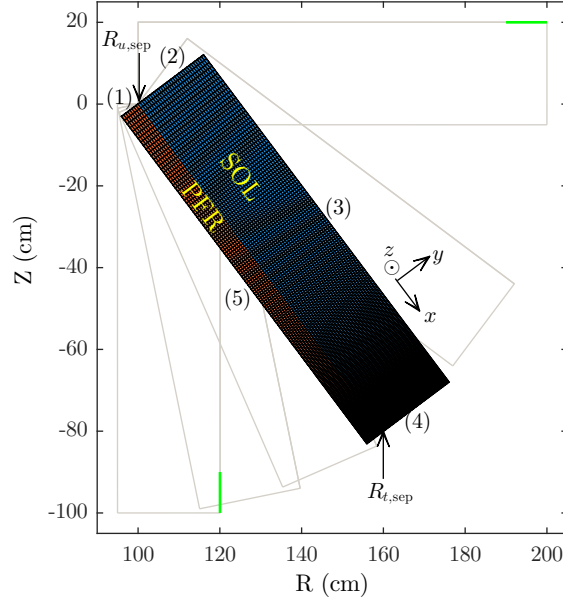
## **2. Simulation setup**

### *2.1. Grids*

In order to isolate the effect of varying total flux expansion, SOLPS-5.0 simulations were run on grids with a minimally complex, rectangular geometry, which spanned a single isolated divertor leg. By rotating these grids about the X-point and fixing the boundary conditions at the upstream divertor entrance (section 2.3), a clean scan was obtained, in which only the total flux expansion changed.

The simulation geometry is shown in figure 1, with poloidal, radial and toroidal directions labelled  $x$ ,  $y$  and  $z$ , respectively, and with vertical and major radius coordinates labelled  $Z$  and  $R$ . Note that although rectangular in the poloidal plane, this is not a slab geometry; the toroidal direction is truly toroidal. The B2.5 (plasma fluid) grids were of size  $n_x = 200$  by  $n_y = 40$ . All cells were perfectly rectangular. Cells were spaced evenly in the radial direction (with  $dy = 6$  mm everywhere) and squeezed poloidally towards the target (with  $dx = 1.5$  mm at the target). The EIRENE walls coincided with the edges of the B2.5 grids. The grid dimensions and magnetic field were chosen to be similar to MAST-U values, as follows. The poloidal distance from the

X-point (positioned at  $R = 1$  m,  $Z = 0$ ) to the target was 1 m and the radial distance across the grid was 0.25 m. For the toroidal magnetic field we made a MAST-U-like assumption that  $B_z = \alpha_z/R$  (with  $\alpha_z = 0.5$  Tm), while for the poloidal magnetic field, given by  $B_x = \alpha_x/R$  (with  $\alpha_x = 0.025$  Tm), we also chose to have a  $1/R$  dependence so as to conserve poloidal flux on the orthogonal grid. There was no radial magnetic field. The resulting parallel connection length from X-point to target was  $L = 20$  m.



**Figure 1.** Minimally complex, isolated divertor leg grid for the  $f_R = 1.6$  case. Other grids, outlined in grey, were created by rotation about the X-point, keeping poloidal flux expansion fixed at unity and the parallel connection length fixed at  $L = 20$  m. The boundary conditions for surfaces (1)-(5) are given in section 2.3. The toroidally symmetric pumping surfaces used for the density ramps to detachment, described in section 4, are shown in green. Colour version available online.

The highlighted grid in figure 1 is for the particular  $f_{R,\text{sep}} = R_{t,\text{sep}}/R_{u,\text{sep}} = 1.6$  case (henceforth we drop the ‘sep’ notation from  $f_R$  since we only analyse flux rings near the separatrix, for which  $f_R \approx f_{R,\text{sep}}$  to within 1%). A regularly spaced six-point scan in  $f_R$  from  $f_R = 1$  to  $f_R = 2$  was carried out by rotating the grid about the fixed X-point, resulting in the other grids used in this study (outlined in grey) in figure 1.

The deliberate simplification of the geometry outlined above ensured that the poloidal flux expansion (fixed at unity), connection length, target angle to the poloidally projected magnetic field, pitch angle and neutral geometry all remained constant across all of the grids used here. Variation in these confounding variables would have been unavoidable in a scan over  $f_R$  using more realistic geometries, making interpretation of the results more difficult. The only relevant quantity that changes in our simplified  $f_R$  scan is  $f_R$  itself.

## 2.2. Equations

In the absence of currents, drifts and impurities and with the particular (simplifying) code input parameters chosen for these simulations, the plasma equations solved here are as follows (see also Schneider *et al* 2006 and Dekeyser *et al* 2011). Particle conservation is given by

$$\frac{\partial n}{\partial t} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} n u_x \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} n u_y \right) = S_{\text{part}}^{\text{neut}}, \quad (1)$$

where  $n = n_e = n_i$  is the pure deuterium plasma density,  $u_x = b_x u_{\parallel}$  is the poloidal projection of the parallel plasma velocity  $u_{\parallel}$ ,  $b_x = B_x/B$  is the sine of the pitch angle,  $u_y = -\frac{D_y^n}{n} \frac{1}{h_y} \frac{\partial n}{\partial y}$  is the radial plasma velocity,  $D_y^n$  is the prescribed anomalous radial particle diffusivity,  $S_{\text{part}}^{\text{neut}}$  is the particle source due to neutrals,  $h_x = 1/|\nabla x|$ ,  $h_y = 1/|\nabla y|$ ,  $\sqrt{g} = h_x h_y h_z$  and  $h_z = 2\pi R$  are the metric coefficients. Conservation of parallel momentum is given by

$$\begin{aligned} \frac{\partial}{\partial t} (m n u_{\parallel}) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} m n u_x u_{\parallel} - \frac{\sqrt{g}}{h_x^2} \frac{4}{3} b_x \eta_{\parallel}^i \frac{\partial u_{\parallel}}{\partial x} \right) \\ + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} m n u_y u_{\parallel} - \frac{\sqrt{g}}{h_y^2} \eta_y^i \frac{\partial u_{\parallel}}{\partial y} \right) = -\frac{b_x}{h_x} \frac{\partial p}{\partial x} + S_{\text{mom}}^{\text{neut}}, \end{aligned} \quad (2)$$

where  $m$  is the deuterium ion mass,  $\eta_{\parallel}^i$  is the Balescu parallel ion viscosity (Balescu 1988),  $\eta_y^i = m n D_y^n$  is the radial viscosity,  $p = n(T_e + T_i)$  is the static pressure,  $T_e$  is the electron temperature,  $T_i$  is the ion temperature and  $S_{\text{mom}}^{\text{neut}}$  is the parallel momentum source due to neutrals. The internal electron energy equation is given by

$$\begin{aligned} \frac{\partial}{\partial t} \left( \frac{3}{2} n T_e \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} (\sqrt{g} h_x \tilde{q}_{ex}) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} \tilde{q}_{ey} \right) = -\frac{n T_e}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} u_x \right) \\ - k_{eq} (T_e - T_i) + S_{\text{eIE}}^{\text{neut}}, \end{aligned} \quad (3)$$

where  $\tilde{q}_{ex} = \frac{3}{2} n u_x T_e - \frac{1}{h_x} \kappa_x^e \frac{\partial T_e}{\partial x}$  is the poloidal electron internal energy flux density,  $\kappa_x^e$  is the Balescu electron heat conductivity (Balescu 1988),  $\tilde{q}_{ey} = \frac{5}{2} n u_y T_e - \frac{1}{h_y} n \chi_y^e \frac{\partial T_e}{\partial y}$  is the radial electron internal energy flux density,  $\chi_y^e$  is the prescribed anomalous radial electron heat diffusivity,  $k_{eq}$  is the equilibration coefficient (Dekeyser *et al* 2011) and  $S_{\text{eIE}}^{\text{neut}}$  is the electron internal energy source due to neutrals. Finally, the ion internal energy equation is given by

$$\begin{aligned} \frac{\partial}{\partial t} \left( \frac{3}{2} n T_i \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} \tilde{q}_{ix} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} \tilde{q}_{iy} \right) = -\frac{n T_i}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} u_x \right) \\ + k_{eq} (T_e - T_i) + \frac{4}{3} b_x \eta_x^i \left( \frac{1}{h_x} \frac{\partial u_{\parallel}}{\partial x} \right)^2 + \eta_y^i \left( \frac{1}{h_y} \frac{\partial u_{\parallel}}{\partial y} \right)^2 + S_{\text{iIE}}^{\text{neut}}, \end{aligned} \quad (4)$$

where  $\tilde{q}_{ix} = \frac{3}{2} n u_x T_i - \frac{1}{h_x} \kappa_x^i \frac{\partial T_i}{\partial x}$  is the poloidal ion internal energy flux density,  $\kappa_x^i$  is the Balescu ion heat conductivity (Balescu 1988),  $\tilde{q}_{iy} = \frac{5}{2} n u_y T_i - \frac{1}{h_y} n \chi_y^i \frac{\partial T_i}{\partial y}$  is the radial ion internal energy flux density,  $\chi_y^i$  is the prescribed anomalous radial ion heat diffusivity and  $S_{\text{iIE}}^{\text{neut}}$  is the ion internal energy source due to neutrals. The source terms due to neutrals in equations (1)-(4) were calculated by the 1999 version of EIRENE (Reiter

2005). All of the reactions listed in table 1 of (Kotov *et al* 2008) were included. In all that follows, subscript 'u' refers to upstream values at the divertor entrance and subscript 't' refers to values at the target.

### 2.3. Boundary conditions

The simplified geometry outlined above allows us to specify boundary conditions at the divertor entrance. The upstream radial energy flux density profile that the divertor has to exhaust, as well as the upstream radial density profile, can therefore be kept fixed throughout the scan in  $f_R$  (note that ensuring the same divertor entrance profiles across the  $f_R$  scan would be very difficult if the divertor leg were not isolated).

The distinction between the private flux region (PFR) and the scrape-off layer (SOL) region, separated by the separatrix at  $y = y_{\text{sep}}$ , was modelled by choosing different boundary conditions on surfaces (1) and (2) of the upstream boundary. These surfaces are labelled in figure 1 and run from  $y = y_{\text{sep}} - \Delta y_{\text{PFR}}$  to  $y = y_{\text{sep}}$  for the upstream PFR surface (1) and from  $y = y_{\text{sep}}$  to  $y = y_{\text{sep}} + \Delta y_{\text{SOL}}$  for upstream SOL surface (2), with  $\Delta y_{\text{SOL}} = 4\Delta y_{\text{PFR}} = 20$  cm chosen. On boundary (1) we assumed  $\partial n_u / \partial x = u_{xu} = \tilde{q}_{exu} = \tilde{q}_{ixu} = 0$  to mimic perfectly symmetric inner and outer PFRs with a stagnation point at the X-point. On boundary (2) we assumed  $n_u = n_{u,\text{sep}} \exp(-(y - y_{\text{sep}})/\lambda_n)$ ,  $\partial u_{xu} / \partial x = 0$  and  $\tilde{q}_{exu} = \tilde{q}_{ixu} = \tilde{q}_{u,\text{sep}} \exp(-(y - y_{\text{sep}})/\lambda_q)$ , with  $n_{u,\text{sep}}$ ,  $\lambda_n$ ,  $P_{\text{in}} \equiv \int_{y_{\text{sep}}}^{y_{\text{sep}} + \Delta y_{\text{SOL}}} (\tilde{q}_{exu} + \tilde{q}_{ixu}) dy$  and  $\lambda_q$  specified as input parameters. Neutrals that reached the upstream boundary (either surface (1) or (2)) were removed from the simulation domain; we assumed that such neutrals were subsequently ionised and transported in the main plasma in such a way as to set up the prescribed upstream plasma boundary conditions.

At the radial walls we assumed a zero radial flux of plasma particles, plasma parallel momentum and plasma internal energy. At the target we set  $u_{\parallel t} \geq c_{st}$  (where  $c_{st}$  is the target sound speed),  $\tilde{q}_{ext} = \gamma_e n_t u_{xt} T_{et}$  (with  $\gamma_e = 4$ ),  $\tilde{q}_{ixt} = \gamma_i n_t u_{xt} T_{it}$  (with  $\gamma_i = 3/2$ ) and assumed an extrapolation boundary condition for  $n_t$ . Both ions and neutrals incident on the target were recycled as deuterium molecules with a recycling fraction  $F_{\text{recyc}}$ . At the radial walls and target, deuterium neutrals were reflected according to a reflection model parameterised by the TRIM code (Eckstein *et al* 1987). In practice this means that most D atoms and D<sub>2</sub> molecules thermally desorb from the walls as D<sub>2</sub> molecules with an energy associated with the wall temperature (assumed to be 300 K here). To mimic active pumping, a fraction  $F_{\text{pump}}$  of neutrals incident on the green surfaces shown in figure 1 (on the  $f_R = 1$  and  $f_R = 2$  grids) could also be removed. The simulations were evolved until, in steady state, the convective plasma flux coming in through the divertor entrance (surfaces (1) and (2)) was equal to the total pumped flux.

### 3. Attached plasmas; results and analysis

#### 3.1. Scaling of target density and temperature with total flux expansion; comparison to the modified two-point model

The original two-point model (2PM) (Stangeby 2000) was modified in (Petrie *et al* 2013) to account for variations in  $f_R$ . This model, presented in the appendix of (Petrie *et al* 2013) and referred to henceforth as the ‘modified 2PM’, predicts the following analytic scalings for  $n_t$  and  $T_{et}$  with  $f_R$ :

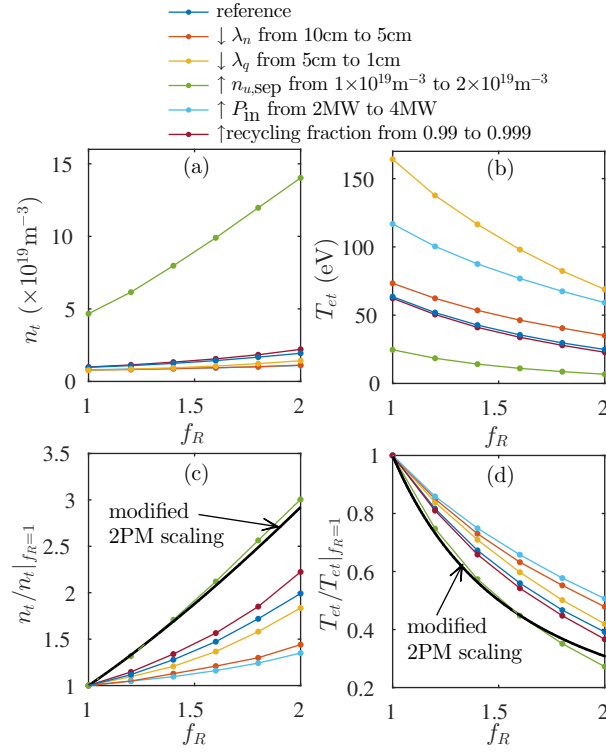
$$n_t \propto f_R^2 \left[ \frac{\ln f_R}{f_R - 1} \right]^{6/7}, \quad (5)$$

$$T_{et} \propto \frac{1}{f_R^2} \left[ \frac{\ln f_R}{f_R - 1} \right]^{-4/7}. \quad (6)$$

A range of SOLPS simulations were run to steady-state in order to test the validity of these scalings across a wide range of parameter space. Input parameters were chosen such that the target plasma remained attached (in terms of both target ion flux and target density rollover, as well as  $T_{et}$  remaining above 5 eV) across the whole range of  $f_R$  for all of the scans presented in this section. For the reference scan over  $f_R$  we set  $D_y^n = \chi_y^e = \chi_y^i = 1 \text{ m}^2\text{s}^{-1}$ ,  $\lambda_n = 10 \text{ cm}$ ,  $\lambda_q = 5 \text{ cm}$ ,  $n_{u,\text{sep}} = 1 \times 10^{19} \text{ m}^{-3}$ ,  $P_{\text{in}} = 2 \text{ MW}$ ,  $F_{\text{recyc}} = 0.99$  and  $F_{\text{pump}} = 0$ . These values for  $\lambda_n$  and  $\lambda_q$  are consistent with fall off lengths at the outer mid-plane of MAST (Kirk *et al* 2004, Thornton *et al* 2014), assuming a realistic poloidal flux expansion of  $\sim 10$  from the outer mid-plane to the divertor entrance. From this reference scan, additional scans were run in which: (i)  $\lambda_n$  was decreased to 5 cm, (ii)  $\lambda_q$  was decreased to 1 cm, (iii)  $n_{u,\text{sep}}$  was increased to  $2 \times 10^{19} \text{ m}^{-3}$ , (iv)  $P_{\text{in}}$  was increased to 4 MW, (v)  $F_{\text{recyc}}$  was increased to 0.999 (i.e. a factor 10 decrease in the pumping speed).

Figures 2a and 2b show the resulting absolute values of  $n_t$  and  $T_{et}$  as a function of  $f_R$  for all of these scans, demonstrating the range of  $n_t$  and  $T_{et}$  that was covered. For each scan, we have taken the target values at the position of maximum target internal energy flux density (for different scans this position could vary from the first to the third SOL ring, i.e. between 0.3 and 1.6 cm from the separatrix, but within each scan the position of this maximum did not change). The same data, now normalised to the values at  $f_R = 1$ , are shown in figures 2c and 2d, with the modified 2PM scalings plotted as solid black lines for comparison (note that these two plots were not significantly altered by different choices of radial position). For completeness, in Appendix A.1 we also compare how the target parallel energy flux density in the simulations scales with the total flux expansion.

We find that for the higher density scan, in which  $n_{u,\text{sep}}$  was increased from  $1 \times 10^{19} \text{ m}^{-3}$  to  $2 \times 10^{19} \text{ m}^{-3}$ , the modified 2PM scalings for both  $n_t$  and  $T_{et}$  are almost exactly recovered by SOLPS. For the other scans, however, the SOLPS scalings of  $n_t$  and  $T_{et}$  with  $f_R$  are weaker than those predicted by the modified 2PM. The weakest scaling was obtained for the high power case, in which a doubling of  $f_R$  caused  $n_t$  ( $T_{et}$ ) to increase



**Figure 2.** Simulated  $n_t$  and  $T_{et}$  as a function of  $f_R$  for various simulation scans, as labelled. Values are plotted at the position of maximum target internal energy flux density. (a) and (b) show absolute values while (c) and (d) show the values normalised to the  $f_R = 1$  case, with the modified two-point model scalings (5) and (6) shown for comparison (black lines). Colour version available online.

(decrease) by a factor of just 1.35 (0.51), compared to a factor of 2.92 (0.31) predicted by the modified 2PM. The observed discrepancies between the modified 2PM scaling and those calculated by SOLPS will now be analysed in more detail.

### 3.2. Analysis of deviations from the modified two-point model

In order to understand the discrepancies shown in figure 2 between the modified 2PM scalings and SOLPS, we will use the ‘two-point model formulation’ equations (Stangeby *et al* 2015, Kotov and Reiter 2009). These give the following *exact* expressions for  $n_t$  and  $T_{et}$  at the downstream end of each SOLPS flux ring:

$$n_t = \left[ \frac{\gamma^2}{32m} \right] \left[ \frac{p_{\text{tot},u}^3}{\tilde{q}_{\parallel u}^2} \right] \left[ \frac{(1 - f_{\text{momloss}})^3}{(1 - f_{\text{pwrloss}})^2} \right] \left[ \frac{4}{(1 + T_{it}/T_{et})^2} \right] \left[ \frac{8M_t^2}{(1 + M_t^2)^3} \right] \left[ \left( \frac{B_u}{B_t} \right)^2 \right], \quad (7)$$

$$T_{et} = \left[ \frac{8m}{e\gamma^2} \right] \left[ \frac{\tilde{q}_{\parallel u}^2}{p_{\text{tot},u}^2} \right] \left[ \frac{(1 - f_{\text{pwrloss}})^2}{(1 - f_{\text{momloss}})^2} \right] \left[ \frac{(1 + T_{it}/T_{et})}{2} \right] \left[ \frac{(1 + M_t^2)^2}{4M_t^2} \right] \left[ \left( \frac{B_t}{B_u} \right)^2 \right], \quad (8)$$

where  $\gamma \equiv (\tilde{q}_{ext} + \tilde{q}_{iat}) / (n_t u_{xt} T_{et}) = \gamma_e + \gamma_i T_{it}/T_{et}$  is the total sheath internal energy transmission coefficient,  $p_{\text{tot},u} \equiv p_u + mn_u u_{\parallel u}^2$  is the total (static plus dynamic) upstream pressure,  $\tilde{q}_{\parallel u} \equiv (\tilde{q}_{exu} + \tilde{q}_{ixu}) / b_x$  is the total (ion plus electron) parallel internal energy



flux density entering the top of the considered flux ring,  $M_t \equiv \sqrt{mn_t u_{\parallel i}^2 / p_t}$  is the target Mach number,  $f_{\text{momloss}} = (\int_t^u S_{\text{mom}}^{\text{tot}} dl) / p_{\text{tot},u}$  is the fraction of total pressure lost between the upstream end of the flux ring and the target, and  $f_{\text{pwrloss}} = (\int_t^u S_{\text{IE}}^{\text{tot}} dV) / (s_u^y \tilde{q}_{xu})$  is the fraction of internal energy flux lost along the considered flux ring (here,  $dl = h_x dx / b_x$  is the line length of a cell in the parallel direction,  $dV = \sqrt{g} dx dy$  is the cell volume and  $s^y = (\sqrt{g} / h_x) dy$  is the area seen by poloidal fluxes). The definitions of  $S_{\text{mom}}^{\text{tot}}$  and  $S_{\text{IE}}^{\text{tot}}$  are given in Appendix A.2.

For the purposes of this analysis it is useful to rewrite equations (7) and (8) as

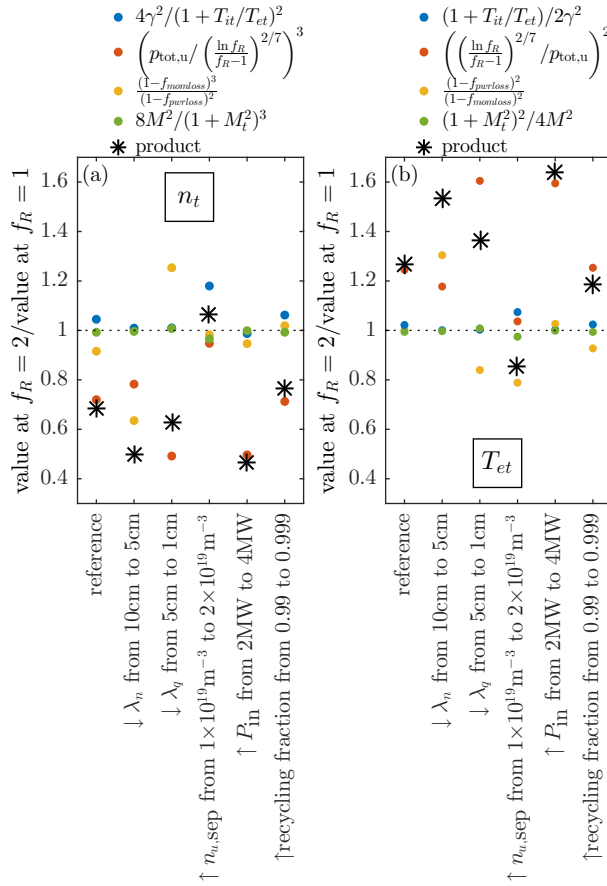
$$n_t = \left[ \frac{1}{32m\tilde{q}_{\parallel u}^2} \right] \left[ \frac{4\gamma^2}{(1 + T_{it}/T_{et})^2} \right] \left[ \left( \frac{p_{\text{tot},u}}{[\ln f_R / (f_R - 1)]^{2/7}} \right)^3 \right] \left[ \frac{(1 - f_{\text{momloss}})^3}{(1 - f_{\text{pwrloss}})^2} \right] \left[ \frac{8M_t^2}{(1 + M_t^2)^3} \right] f_R^2 \left[ \frac{\ln f_R}{f_R - 1} \right]^{6/7}, \quad (9)$$

$$T_{et} = \left[ \frac{8m\tilde{q}_{\parallel u}^2}{e} \right] \left[ \frac{(1 + T_{it}/T_{et})}{2\gamma^2} \right] \left[ \left( \frac{[\ln f_R / (f_R - 1)]^{2/7}}{p_{\text{tot},u}} \right)^2 \right] \left[ \frac{(1 - f_{\text{pwrloss}})^2}{(1 - f_{\text{momloss}})^2} \right] \left[ \frac{(1 + M_t^2)^2}{4M_t^2} \right] \frac{1}{f_R^2} \left[ \frac{\ln f_R}{f_R - 1} \right]^{-4/7}. \quad (10)$$

In this form we can see that the first factors in both (9) and (10) are constant across an  $f_R$  scan, while the last factors are just the modified 2PM scalings (5) and (6). The 2nd to 5th factors therefore represent the additional physics in this SOLPS-5.0 model which is not present in the modified 2PM. If the product of these 2nd to 5th factors varies as a function of  $f_R$  then the simulations will deviate from the modified 2PM scaling. If, however, the assumptions used by (Petrie *et al* 2013) when deriving the modified 2PM are well met (i.e. that  $f_{\text{momloss}} = f_{\text{pwrloss}} = 0$ ,  $T_e = T_i$ ,  $M_t = 1$ ,  $p_{\text{tot},u} = p_u$  and  $T_{eu} \propto [\ln f_R / (f_R - 1)]^{2/7}$  ‡), then the 2nd to 5th factors will not vary with  $f_R$  and SOLPS-5.0 will recover the modified 2PM scaling.

Figure 3a explains the discrepancies between the change in  $n_t$  predicted by the modified 2PM and the change in  $n_t$  predicted by SOLPS, when going from  $f_R = 1$  to  $f_R = 2$ . We plot the values of the 2nd to 5th factors of equation (9) at  $f_R = 2$ , divided by their values at  $f_R = 1$ , on the same flux tubes used in figure 2. These ratios are plotted with different colours for each factor, as given in the legend. This is done for each  $f_R$  scan, as labelled on the  $x$ -axis. For each  $f_R$  scan, the product of the coloured dots is equal to the SOLPS value of  $n_t|_{f_R=2}/n_t|_{f_R=1}$  divided by the modified 2PM value of  $n_t|_{f_R=2}/n_t|_{f_R=1}$ . These products are shown as black asterisks in figure 3a. A value of unity for this asterisk means that SOLPS and the modified 2PM predict the same increase in  $n_t$  when  $f_R$  increases from 1 to 2. A value less (greater) than unity for the asterisk means that SOLPS predicts a smaller (larger) increase in  $n_t$ , i.e. a weaker (stronger) scaling with  $f_R$  than the modified 2PM. To be clear, the asterisks

‡ This last assumption turns out to be important and will be assessed in detail later.



**Figure 3.** Explanation of the discrepancies between the change in  $n_t$  (a) or  $T_{et}$  (b) predicted by the modified 2PM and the change predicted by SOLPS, when going from  $f_R = 1$  to  $f_R = 2$ . Coloured dots show the values of the 2nd to 5th factors in equation (9) (figure a) and equation (10) (figure b) at  $f_R = 2$  divided by their values at  $f_R = 1$ . Asterisks show the product of the coloured dots for each  $f_R$  scan. See text for details. Note that the blue dots are hidden behind the green in the “ $\downarrow \lambda_n$  from 10cm to 5cm” and “ $\downarrow \lambda_q$  from 5cm to 1cm” cases. Colour version available online.

give the factors by which the coloured lines shown previously in figure 2c differ from the solid black line at  $f_R = 2$ . The utility of this exercise is that now the *reasons* for these differences are revealed by the factors that comprise them. In figure 3b, we have carried out the same exercise for the 2nd to 5th factors of equation (10), explaining the discrepancies between the change in  $T_{et}$  predicted by the modified 2PM and the change in  $T_{et}$  predicted by SOLPS, when going from  $f_R = 1$  to  $f_R = 2$ .

We notice from figure 3 that changes in the 2nd and 5th factors in (9) and (10) (due to changes in  $M_t$  and  $T_{it}/T_{et}$  respectively) are small for all of the  $f_R$  scans; these factors play little role in causing discrepancies from the modified 2PM scaling with  $f_R$ . Furthermore, for the high density case, changes in all of the other factors are small as well, so that the high density  $f_R$  scan conforms well to the modified 2PM scaling. In the few cases where the 4th factors in (9) and (10) (due to losses along a flux ring) do change

significantly across the  $f_R$  scan, we found that those changes are dominated by changes in  $f_{\text{momloss}}$  rather than  $f_{\text{pwrloss}}$ . For these attached simulations, changes in  $f_{\text{momloss}}$  come from changes in the parallel viscosity and in the radial divergence of momentum, not from changes in the momentum source due to neutrals. Overall, however, there is no general trend for the 4th factors.

Consider now the 3rd factor in equation (9) for  $n_t$ . The value of this factor at  $f_R = 2$  divided by its value at  $f_R = 1$  (as plotted with red markers in figure 3a) is equal to the value of  $(p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1})^3$  calculated by SOLPS divided by the value of  $(p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1})^3$  predicted by the modified 2PM. Recall that the modified 2PM predicts  $p_{\text{tot},u} \propto [\ln f_R/(f_R - 1)]^{2/7}$ , i.e.  $p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1} = 0.90$ . Therefore, if SOLPS predicts  $p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1} < 0.90$ , then the red marker in figure 3a will sit below one, pushing the SOLPS simulation towards a lower value of  $n_t|_{f_R=2}/n_t|_{f_R=1}$  (i.e. a weaker scaling) than predicted by the modified 2PM. Indeed, this was the case for all of the  $f_R$  scans that produced a weaker scaling of  $n_t$  than the modified 2PM; for those cases the total upstream pressure decreased more strongly with  $f_R$  than expected from the modified 2PM (in fact this was true for all of the scans except the higher density scan – recall also figures 2c).

An analogous argument can also be made for the 3rd factor in equation (10) for  $T_{et}$ , except that the value of this factor at  $f_R = 2$  divided by its value at  $f_R = 1$  (as plotted with red markers in figure 3b) is now equal to the value of  $(p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1})^2$  predicted by the modified 2PM divided by the value of  $(p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1})^2$  calculated by SOLPS. Now, if SOLPS predicts  $p_{\text{tot},u}|_{f_R=2}/p_{\text{tot},u}|_{f_R=1} < 0.90$ , then the red marker in figure 3b will sit above one, pushing the SOLPS simulation towards a higher value of  $T_{et}|_{f_R=2}/T_{et}|_{f_R=1}$  (i.e. a weaker scaling) than predicted by the modified 2PM. Note that the red marker won't sit as far above one in figure 3b as it sits below one in figure 3a because of the squared exponent in the 3rd factor in (10) compared to the cubed exponent in the 3rd factor of (9). This explains why the SOLPS scalings for  $T_{et}$  are closer to the modified 2PM than the scalings for  $n_t$  (recall also figures 2c and 2d). Given the importance of this stronger-than-expected decrease in upstream pressure with  $f_R$  in the SOLPS simulations, we now consider it further.

### 3.3. Understanding the stronger-than-expected decrease in upstream pressure with total flux expansion

Since  $n_u$  was kept fixed for each scan and since the upstream dynamic pressure was always small compared to the upstream static pressure, a stronger-than-expected decrease in  $p_{\text{tot},u}$  amounts to a stronger-than-expected decrease in  $T_{eu} + T_{iu}$ . Now, consider the following equations for  $T_{eu}$  and  $T_{iu}$ , derived by integrating the electron and ion heat conduction equations along a field line whose major radius varies linearly in the parallel direction (Petrie *et al* 2013):

$$T_{eu} = \left( \frac{7\tilde{q}_{e||u}L}{2\kappa_{0e}} \left[ \frac{\ln f_R}{f_R - 1} \right] + T_{et}^{7/2} \right)^{2/7}, T_{iu} = \left( \frac{7\tilde{q}_{i||u}L}{2\kappa_{0i}} \left[ \frac{\ln f_R}{f_R - 1} \right] + T_{it}^{7/2} \right)^{2/7}, \quad (11)$$

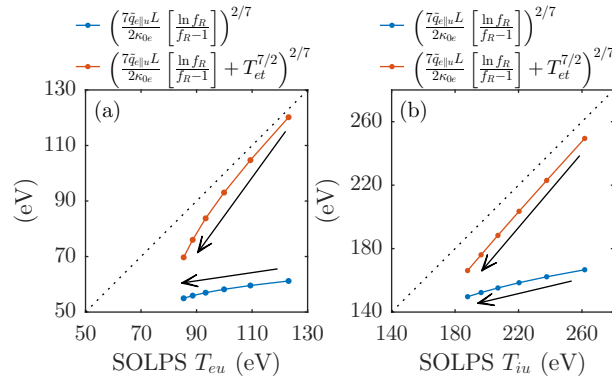
where  $\tilde{q}_{e\parallel u}$  and  $\tilde{q}_{i\parallel u}$  are the electron and ion parallel internal energy flux densities upstream,  $\kappa_{0e} = 2000$  and  $\kappa_{0i} = 60$  are the electron and ion parallel conductivity coefficients, respectively (Stangeby *et al* 2000).

Equations (11) assume that conduction dominates both electron and ion parallel internal energy transport, that  $R$  varies linearly in the parallel direction (which is exactly met on the grids used here), and that there are no losses of electron or ion internal energy along the considered flux ring. Importantly, in order to achieve the modified 2PM scalings (5) and (6), it is also necessary to assume a sufficient drop in temperature along the flux ring so that the target temperature can be neglected (often referred to as the conduction-limited regime). This must be true *throughout the scan over  $f_R$* . If, however, we are in a regime where at any point (or indeed all points) in the  $f_R$  scan the SOL is sheath-limited and the target temperature *cannot* be neglected, then the drop in upstream temperature (and therefore the upstream total pressure) will be larger than predicted by the modified 2PM. As explained in the previous subsection, this means that the SOLPS-calculated  $n_t$  and  $T_{et}$  exhibit a weaker dependence on  $f_R$  than predicted by the modified 2PM§.

To demonstrate this effect, we concentrate on the high power  $f_R$  scan in which  $P_{in}$  was increased from the reference value of 2 MW to 4 MW. As already recognised, this scan exhibits the largest discrepancies in the fractional changes in  $n_t$  and  $T_{et}$  compared to the modified 2PM. However, the effect was observed to lesser extents in all of the  $f_R$  scans which displayed a more conservative scaling for  $n_t$  and  $T_{et}$  compared to the modified 2PM. Figure 4 plots equations (11) (which are estimates of the SOLPS upstream temperatures) as functions of the actual SOLPS-calculated  $T_{eu}$  and  $T_{iu}$  for the high power  $f_R$  scan, both excluding the target temperature terms (blue lines) and including them (red lines). The arrows point in the direction of increasing  $f_R$ .

A good agreement is found between equations (11) and the simulated upstream temperatures when the target temperature is included, suggesting that parallel conduction dominates over convection in the simulation and that internal energy losses from both electrons and ions are small. Importantly, however, when the target temperature is excluded (as assumed in the 2PM), the predicted drop in upstream temperature is much less than was simulated. Note that the blue and red lines almost converge at high  $f_R$ , suggesting that including the target temperature becomes less important, i.e. the simulation moves from the sheath-limited to the conduction-limited regime, as the grid is rotated outwards.

§ In fact, further analysis of figure 2c reveals that the SOLPS scalings with  $f_R$  get closer to the modified 2PM scalings towards the end of the  $f_R$  scan, as the conduction-limited assumption becomes more appropriate. For example, for the high power  $f_R$  scan, an increase in  $f_R$  from 1 to 1.2 gives a factor of just 0.86 decrease in  $T_{et}$ , while the modified 2PM predicts a factor 0.73 decrease. However, an increase in  $f_R$  from 1.8 to 2.0 gives a factor 0.88 decrease in  $n_t$ , which is closer to the modified 2PM prediction of a factor 0.84 decrease.



**Figure 4.** Comparison of equations (11) to the SOLPS-calculated upstream electron (a) and ion (b) temperatures for the high power  $f_R$  scan. Cases where the target temperature is included and excluded are shown, as labelled. Arrows point in the direction of increasing  $f_R$ . Colour version available online.

### 3.4. Effect of total flux expansion on the transition from sheath-limited to conduction-limited regimes

(Kotschenreuther *et al* 2010) extended the two-point analysis of (Stangeby 2000 – equation (4.110)) to find that, for a constant ratio of target to upstream temperatures,  $n_u|_{T_{et}/T_{eu}} \propto \tilde{q}_{e||u}^{4/7} / f_R L^{3/7}$ . Under the assumption that  $R$  varies linearly in the parallel direction (i.e. rearranging the equations in the appendix of (Petrie *et al* 2013), we find a slightly modified version:

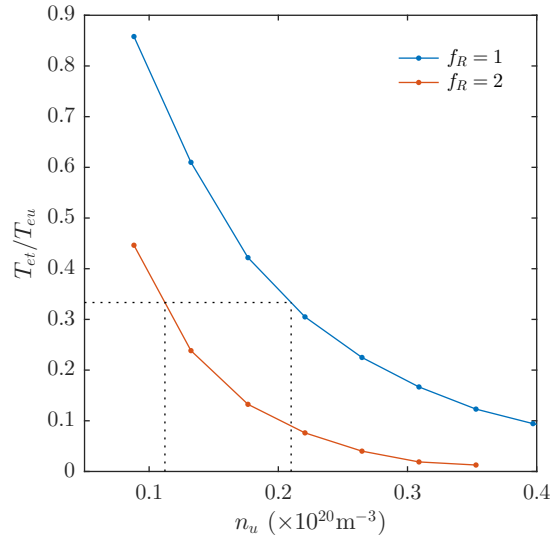
$$n_u|_{T_{et}/T_{eu}} \propto \frac{\tilde{q}_{e||u}^{4/7}}{L^{3/7} f_R} \left( \frac{\ln f_R}{f_R - 1} \right)^{3/7}. \quad (12)$$

An upstream density scan, described in more detail in section 4, was carried out on the  $f_R = 1$  and  $f_R = 2$  grids. Figure 5 plots the resulting  $T_{et}/T_{eu}$  as a function of  $n_u$ . Defining (rather arbitrarily) the transition from sheath-limited to conduction-limited regimes to occur at  $T_{et}/T_{eu} = 1/3$ , we observe that the  $f_R = 2$  case transitions at 0.53 times the density of the  $f_R = 1$  case ( $n_u = 1.12 \times 10^{19} \text{ m}^{-3}$  compared to  $n_u = 2.10 \times 10^{19} \text{ m}^{-3}$ ). This compares well to equation (12), which predicts a factor 0.58 difference. Note that at these low densities the recycling model had no effect on this result.

## 4. Density-driven detachment onset; results and analysis

### 4.1. Rollover as a function of upstream density

In order to understand the effect of total flux expansion on detachment onset, scans in the upstream separatrix density  $n_{u,\text{sep}}$  were performed on an  $f_R = 1$  grid (representing a conventional slot divertor) and on an  $f_R = 2$  grid (representing a Super-X divertor). To assess the sensitivity to the pumping model, the following four pumping models (i.e. combinations of  $F_{\text{recyc}}$  and  $F_{\text{pump}}$ ) were tested on both grids: (i)  $F_{\text{recyc}} = 0.99$ ,  $F_{\text{pump}} = 0$ , (ii)  $F_{\text{recyc}} = 0.999$ ,  $F_{\text{pump}} = 0$ , (iii)  $F_{\text{recyc}} = 1$ ,  $F_{\text{pump}} = 0.01$ , (iv)  $F_{\text{recyc}} = 1$ ,

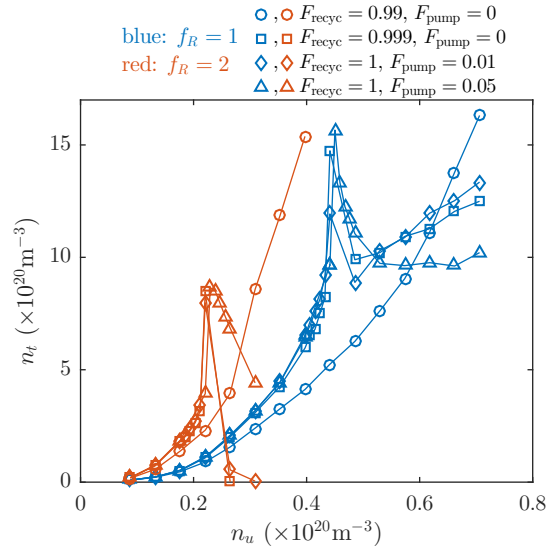


**Figure 5.** Transition from the sheath-limited to conduction-limited regimes as a function of  $n_u$ , for  $f_R = 1$  and  $f_R = 2$ . The interpolated values of  $n_u$  at which  $T_{et} = T_{eu}/3$  are also shown. Colour version available online.

$F_{\text{pump}} = 0.05$ . All other input parameters were kept the same as for the reference case described in section 3.1. We discuss only detachment onset in pure deuterium plasmas driven by an increase in the upstream density; detachment via impurity seeding is left for future work.

Figure 6 shows  $n_t$  as a function of  $n_u$ . For all of the figures in this section, values were taken at the radial position where the target internal energy flux density ( $\tilde{q}_{ixt} + \tilde{q}_{ext}$ ) was maximum for the lowest density cases (at  $y = y_{\text{sep}} + 1.6$  cm, corresponding to the third SOL ring). Plots are made for  $f_R = 1$  (blue markers) and  $f_R = 2$  (red markers) and for each pumping model (distinguished by different marker shapes, as labelled). We observe that, when  $n_t$  does roll over, it does so at approximately half the upstream density when the total flux expansion is doubled ( $n_u = 2.3 \times 10^{19} \text{ m}^{-3}$  at rollover for  $f_R = 2$  compared to  $n_u = 4.5 \times 10^{19} \text{ m}^{-3}$  at rollover for  $f_R = 1$ ). Furthermore, the value of  $n_t$  at rollover for  $f_R = 2$  is approximately half its value at rollover for  $f_R = 1$  ( $n_t = 8.5 \times 10^{20} \text{ m}^{-3}$  at rollover for  $f_R = 2$  compared to  $n_t = 16.2 \times 10^{20} \text{ m}^{-3}$  at rollover for  $f_R = 1$ ).

As a side note, we also observe from figure 6 that the pumping model *can* influence the target plasma response to increasing upstream density. In particular, at high densities, the cases where pumping occurs entirely at the target via a recycling fraction  $F_{\text{recyc}} = 0.99$  (open circles) exhibit a different trend with  $n_u$  to the other pumping models. On the  $f_R = 1$  grid there was no rollover in  $n_t$  for this pumping model, across the entire range of (physically reasonable) upstream densities investigated. On the  $f_R = 2$  grid for  $n_u > 4 \times 10^{19} \text{ m}^{-3}$ , the target oscillated between attached and detached solutions (not shown in figure 6). Although an explanation of this behaviour is beyond the scope of this paper, we present it here because it is typically assumed



**Figure 6.** Target plasma density as a function of the upstream separatrix plasma density for the  $f_R = 1$  (conventional) grid (blue) and the  $f_R = 2$  (Super-X) grid (red), and for different pumping models (labelled with different marker shapes). Colour version available online.

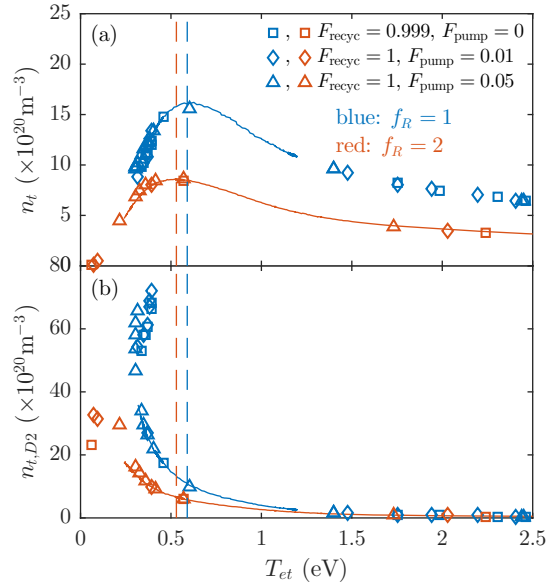
that the pumping model does not affect the target plasma as long as the recycling flux is dominant (Chankin *et al* 2006). The reason why we do see an effect of the pumping model even though the recycling flux is dominant will be a topic of future work. We concentrate here on the three other pumping models which all exhibit a similar rollover behaviour as a function of upstream density.

#### 4.2. Rollover as a function of target temperature

Figure 7a shows  $n_t$  as a function of  $T_{et}$  for the three pumping models which did exhibit a rollover on both grids. The markers denote steady-state simulations, while the solid lines show the time-dependent path taken by simulations in which the density was increased from an upstream density just before rollover to an upstream density just after rollover (for the  $F_{recyc} = 0.999$ ,  $F_{pump} = 0$  pumping model). This path is seen to be consistent with the steady state simulations and enabled us to capture more accurately the target electron temperature at which  $n_t$  rolled over.

For both  $f_R = 1$  and  $f_R = 2$ , the value of  $T_{et}$  at which the rollover occurred was very similar:  $T_{et} = 0.59$  eV at rollover on the  $f_R = 1$  grid and  $T_{et} = 0.53$  eV at rollover on the  $f_R = 2$  grid (note that we define target values at the interface between the last grid cell and the guard cell; at the centre of the last grid cell  $T_e$  was 0.73 eV at rollover on the  $f_R = 1$  grid and 0.83 eV at rollover on the  $f_R = 2$  grid). These temperatures are labelled with vertical dashed lines in figure 7. Given this, the fact that  $n_t$  rolls over at approximately half the value of  $n_u$  for twice the value of  $f_R$  is entirely consistent with the modified 2PM; equation (A13) in (Petrie *et al* 2013) predicts that

$n_u \propto \frac{1}{\sqrt{T_{et}}} \frac{1}{f_R} \left[ \frac{\ln f_R}{f_R - 1} \right]^{-2/7}$ . Also, equation (A12) in (Petrie *et al* 2013) predicts that  $n_t \propto \frac{1}{T_{et}^{3/2}} \frac{1}{f_R}$ , in line with the value of  $n_t$  at rollover on the  $f_R = 2$  grid being half the value of  $n_t$  at rollover on the  $f_R = 1$  grid, given that the rollover occurs at the same target temperature.



**Figure 7.** Target plasma density (a) and target molecular density (b) as functions of the target electron temperature during upstream-density-driven detachment. Colours and marker are the same as figure 6. Colour version available online.

We hypothesise that the target temperature at rollover is the same in both cases because this is the target temperature at which the the molecular density rises strongly (presumably due to a rapid decrease in the molecular dissociation rate) and elastic collisions with molecules are able to remove sufficient parallel momentum from the ions in order to induce a rollover (our preliminary analysis suggests that recombination indirectly acts as a momentum sink by creating atoms which subsequently recycle as molecules and undergo elastic collisions with ions, rather than directly removing ion momentum in the recombination event itself). This hypothesis will be investigated further in a forthcoming paper. We note here that, as shown in figure 7b, a steep rise in the target molecular density (at the last cell of the third SOL ring) was observed, beginning at the same value of  $T_{et}$  at which  $n_t$  rolled over. This is consistent with the important role of  $D_2$  molecules previously reported by (Kotov and Reiter 2009).

## 5. Conclusions and future work

In this work, by operating SOLPS-5.0 in a minimally complex geometry, we have isolated and assessed the role of total flux expansion on the target plasma. Modelling only a single isolated slot divertor leg, we have demonstrated that at upstream densities for



which the SOL remains in the attached, conduction-limited regime throughout the scan in  $f_R$ , the scalings of  $n_t$  and  $T_{et}$  with  $f_R$  predicted by SOLPS-5.0 (in the absence of currents, drifts and impurities) are well reproduced by the modified 2PM (Petrie *et al* 2013). If, however, the SOL is sheath-limited for any of the  $f_R$  scan, then the increase (decrease) in  $n_t$  ( $T_{et}$ ) with  $f_R$  reported by SOLPS-5.0 is significantly weaker than predicted by the modified 2PM scaling.

This result is particularly important when considering, for a given tokamak plasma, how much you would need to increase the total flux expansion in order to reach a given target temperature (at which, for example, you would expect the target to detach or the physical sputtering to reduce). If that given plasma is in the sheath limited regime, then the required increase in total flux expansion would be more than predicted by the modified 2PM, and some other model (such as SOLPS-5.0) is required to predict how much more.

Upstream density scans were carried out on the  $f_R = 1$  and  $f_R = 2$  grids. The transition from sheath-limited to conduction-limited regimes was seen to occur at approximately half the upstream density on the  $f_R = 2$  grid compared to the  $f_R = 1$ , in good agreement with the modified 2PM prediction (equation (12)).

As the upstream density was increased further, we found that the target plasma became sensitive to the particular pumping model used. In particular, simulations where pumping was implemented via a target recycling coefficient of 0.99 failed to roll over at densities up to twice those at which simulations with the other tested pumping models did roll over. The other three pumping models tested did detach at very similar upstream densities, however.

Importantly, the target electron density was found to roll over at almost the same target electron temperature on both  $f_R = 1$  and  $f_R = 2$  grids. Given this, the modified 2PM predicts that both the upstream plasma density required for rollover, as well as the target plasma density at which rollover occurs, should be halved when  $f_R$  is doubled. This is indeed what was observed in the simulations. We have hypothesised that the rollover in target density occurs at such similar target temperatures because of the sharp increase in molecular density that occurs at that temperature (presumably because of a decrease in the molecular dissociation rate), allowing molecular elastic scattering to remove ion parallel momentum and thereby induce rollover.

As well as testing the above hypothesis, future work will assess the role of impurities in density-driven detachment, as well as impurity-driven detachment. We will also assess the stability of the detachment front once it has pulled off from the target and investigate the detachment window of upstream density in which the detachment front remains below the X-point.

## Appendix

### Appendix A.1. Scaling of the total parallel energy flux density at the target with $f_R$

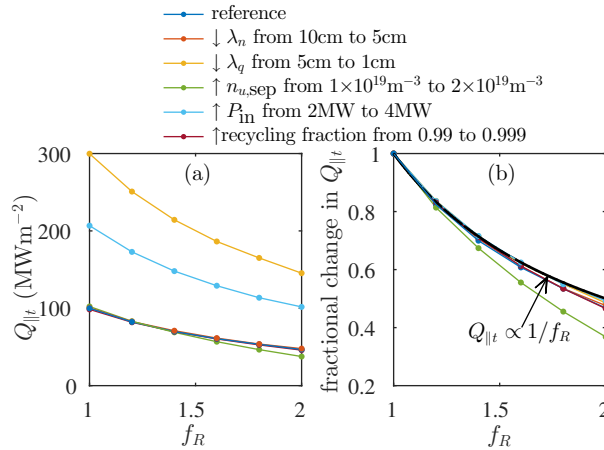
In the case that the integrated energy loss along each flux tube does not vary with total flux expansion, we expect the total parallel energy flux density at the target to vary simply as

$$Q_{\parallel t} \propto \frac{1}{f_R}, \quad (\text{A.1})$$

where  $Q_{\parallel t} = \frac{5}{2}nu_{\parallel}T_e - \frac{1}{h_x b_x} \kappa_x^e \frac{\partial T_e}{\partial x} + \frac{5}{2}nu_x T_i - \frac{1}{h_x b_x} \kappa_x^i \frac{\partial T_i}{\partial x} + \frac{1}{2}mnu_{\parallel}^3$  is the *total* parallel energy flux density at the target.

Figure A1a shows the absolute value of  $Q_{\parallel t}$  for all of the  $f_R$  scans described in section 3.1. As in figure 2, for each  $f_R$  scan, values were taken at the radial location where the target internal energy flux density was maximum; this position did not change throughout each individual scan. These locations coincided with the maximum *total* parallel energy flux density at the target, so that figure A1a actually shows the peak value of  $Q_{\parallel t}$ . Figure A1b shows the same data plotted as a fractional change from the  $f_R = 1$  case.

We observe that the simulations show an excellent agreement to the expected  $Q_{\parallel t} \propto \frac{1}{f_R}$  (black line). The slight exception to this is the higher density case, for which  $Q_{\parallel t}$  decreased somewhat faster with increasing  $f_R$  than expected. We attribute this to an increase in  $S_{\text{IE}}^{\text{tot}}$  along the considered flux tube, from 0.38 in the  $f_R = 1$  case to 0.57 in the  $f_R = 2$  case. This in turn is primarily due to a factor three increase in the  $\text{D}\alpha$  radiation for the  $f_R = 2$  case. Physically, as  $f_R$  is increased in the higher density  $f_R$  scan, the target electron temperature becomes sufficiently low that  $\text{D}\alpha$  radiation becomes significant, resulting in a slightly stronger scaling than  $Q_{\parallel t} \propto \frac{1}{f_R}$ .



**Figure A1.** Simulated peak  $Q_{\parallel t}$  as a function of  $f_R$  for the same simulation scans described in section 3.1. (a) shows absolute values while (b) shows the fractional changes relative to the  $f_R = 1$  case, with the scaling  $Q_{\parallel t} \propto \frac{1}{f_R}$  shown for comparison (black line). Colour version available online.

Appendix A.2. Definitions of  $S_{\text{mom}}^{\text{tot}}$  and  $S_{\text{IE}}^{\text{tot}}$ 

Rearranging the steady-state parallel momentum equation (2) and integrating from target to divertor entrance gives the following equation for total pressure balance:

$$p_{\text{tot},u} - p_{\text{tot},t} = \int_t^u S_{\text{mom}}^{\text{tot}} dl, \quad (\text{A.2})$$

where

$$S_{\text{mom}}^{\text{tot}} = S_{\text{mom}}^{\text{neut}} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x^2} \frac{4}{3} b_x \eta_{\parallel}^i \frac{\partial u_{\parallel}}{\partial x} \right) - \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} m n u_y u_{\parallel} - \frac{\sqrt{g}}{h_y^2} \eta_y^i \frac{\partial u_{\parallel}}{\partial y} \right) - \frac{m n u_{\parallel}^2}{\sqrt{g}} \frac{\partial}{\partial x} (dA_{\parallel}) \quad (\text{A.3})$$

and  $dA_{\parallel} = s^y b_x$  is the flux tube area normal to the magnetic field. Also, adding equations (3) and (4) in the steady-state and integrating gives the following equation for total internal energy flux balance:

$$s_u^y (\tilde{q}_{exu} + \tilde{q}_{ixu}) - s_t^y (\tilde{q}_{ext} + \tilde{q}_{ixt}) = \int_t^u S_{\text{IE}}^{\text{tot}} dV, \quad (\text{A.4})$$

where

$$S_{\text{IE}}^{\text{tot}} = S_{\text{elIE}}^{\text{neut}} + S_{\text{iiIE}}^{\text{neut}} - \frac{1}{\sqrt{g}} \frac{\partial}{\partial y} \left( \frac{\sqrt{g}}{h_y} (\tilde{q}_{ey} + \tilde{q}_{iy}) \right) - \frac{n T_e}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} u_x \right) - \frac{n T_i}{\sqrt{g}} \frac{\partial}{\partial x} \left( \frac{\sqrt{g}}{h_x} u_x \right) - \frac{4}{3} b_x \eta_x^i \left( \frac{1}{h_x} \frac{\partial u_{\parallel}}{\partial x} \right)^2 - \eta_y^i \left( \frac{1}{h_y} \frac{\partial u_{\parallel}}{\partial y} \right)^2 \quad (\text{A.5})$$

Rearranging (A.2) and (A.4) and using the boundary condition on internal energy flux density at the target then yields equations (7) and (8) (Stangeby *et al* 2015). This procedure is similar to the one described in (Kotov and Reiter 2009), except that here we balance total pressure  $p_{\text{tot}}$ , resulting in a geometric term  $-\frac{m n u_{\parallel}^2}{\sqrt{g}} \frac{\partial}{\partial x} (dA_{\parallel})$  in  $S_{\text{mom}}^{\text{tot}}$ , while (Kotov and Reiter 2009) balanced total *force*  $b_x s^y p_{\text{tot}}$ , resulting in a geometric term  $\frac{p}{\sqrt{g}} \frac{\partial}{\partial x} (dA_{\parallel})$  in  $S_{\text{mom}}^{\text{tot}}$ . The latter term cannot be ignored in the force balance for a super-X divertor, while the former typically can. This is because  $p$  tends to be non-negligible along the entire SOL whereas  $u_{\parallel}$  generally only rises over a small region close to the target. The other difference from (Kotov and Reiter 2009) is that we are balancing internal energy fluxes while they balanced total energy fluxes. This results in the third and fourth terms in (A.5) which were not present previously. In our simulations these terms do not typically play a significant role.

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this paper please contact [PublicationsManager@ccfe.ac.uk](mailto:PublicationsManager@ccfe.ac.uk). The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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