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Using EDGE2D-EIRENE to simulate the effect of impurity seeding and fueling on the upstream electron separatrix temperature

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1. Introduction

The separatrix temperature is required as an input for several models of the tokamak edge. For example, the heuristic power decay length ($\lambda_q$) model in reference [1], H-mode density limit studies in reference [2] and pedestal stability analysis [3]. In these models the fundamental equation used to approximate the separatrix temperature is the two point model equation [4]:

$$T_{eu,sep} = \left( \frac{7\lambda_{q,sep}}{2\kappa} \right)^{\frac{2}{3}}$$

(1)

Here, $T_{eu,sep}$ is the upstream electron temperature (eV), which is taken at the low field side (LFS) midplane separatrix. $q_{\parallel,sep}$ is the total heat flux (assuming that the ion heat flux is small) at the entrance to the divertor on the LFS at the separatrix. $P_{sep}$ is the power crossing the separatrix ($\text{Wm}^{-2}$), $L$ is the connection length (m) and $\kappa = 2000$ (Wm$^{-2}$eV$^{-2}$).

Practically the models referenced above use the following equation to approximate $T_{eu,sep}$ because it contains experimentally measurable variables unlike $q_{\parallel,sep}$: To derive this equation the approximation $q_{\parallel,sep} \sim (P_{sep}/2)/A_k$ is applied to Eq. (1) to yield [4]:

$$T_{eu,sep} = \left( \frac{7((P_{sep}/2)/A_k)L}{2\kappa} \right)^{\frac{2}{3}}$$

(2)

Here, $P_{sep}$ is power crossing the last closed flux surface from the
Table 1
The markers used to represent the parameters in the simulation scan are shown in this table. Blue markers are neon seeding, green markers are nitrogen seeding and black are unseeded. The size of the symbol represents an increase in separatrix electron density ($n_{e,\text{sep}}$). The different types of the symbol are to represent different impurity radiation powers. The open symbols represent simulations which have had the impurity radiation in the main SOL (above the x-point) removed from the total radiation of the simulation. The colour, shape and size of the open symbol retain the same meaning as the closed symbols.

<table>
<thead>
<tr>
<th>$n_{e,\text{sep}}$</th>
<th>Impurity radiation ($P_{\text{rad}}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0 MW</td>
</tr>
<tr>
<td></td>
<td>Neon</td>
</tr>
<tr>
<td>2x10$^{19}$ m$^{-3}$</td>
<td>o</td>
</tr>
<tr>
<td>2.5x10$^{19}$ m$^{-3}$</td>
<td>o</td>
</tr>
<tr>
<td>3x10$^{19}$ m$^{-3}$</td>
<td>o</td>
</tr>
</tbody>
</table>

confined plasma (W) and

$$A_q = 2\pi R_A \left( \frac{B_x}{B} \right)$$

(3)

where $A_q$ is the area perpendicular to a (toroidally extended) flux tube of width $\lambda_q (m)$ that $P_{\text{rad}}$ falls over, $\lambda_q$ is the power decay width at the upstream position, $R(m)$ is the radius at the upstream position, and $\left( \frac{B}{B} \right)$ is the ratio of the poloidal magnetic field to the total magnetic field at the upstream location. Note that Eq. (2) assumes no power loss between the x-point and the upstream position (low field side mid-plane separatrix).

From Eq. (2) two scalings between the $T_{\text{e,sep}}$ and $P_{\text{rad}}$ can be derived; (1) $T_{\text{e,sep}} \propto P_{\text{rad}}^2$, which is derived assuming that $P_{\text{rad}}$ is only significantly varying parameter and, (2) $T_{\text{e,sep}} \propto P_{\text{rad}}^x$ which is derived assuming that $\lambda_q$ in Eq. (2) can be calculated as a competition between conductive parallel heat transport and prescribed radial diffusive heat transport, in which case $\lambda_q \propto P_{\text{rad}}^2$ (Equation (5.77) from reference [4]).

$T_{\text{e,sep}}$ is a boundary condition for pedestal stability analysis codes [5]. The weak power dependence of $P_{\text{rad}}$ from the scaling $T_{\text{e,sep}} \propto P_{\text{rad}}^2$ is often used to justify the assumption that the variation in $T_{\text{e,sep}}$ can be neglected [5]. So, a value of 100-eV is often assumed as the $T_{\text{e,sep}}$ boundary condition for pedestal stability analysis for the JET, independent of the specifics of a particular JET discharge.

Work presented in references [6,7] considered the effect of nitrogen seeding using EDGE2D-EIRENE. However, the authors focused on the effect on the divertor and comparison to experiment rather than the upstream effects examined in this paper.

In this work the applicability of Eq. (2) and the variation in $T_{\text{e,sep}}$ was assessed using the edge fluid neutral code EDGE2D-EIRENE [8-10]. Simulations were conducted with varying neon and nitrogen seeding radiation and a range of electron separatrix densities ($n_{e,\text{sep}}$). The effect of neon seeding on $T_{\text{e,sep}}$ has not been examined previously. Impurities, either intrinsically sputtered or injected deliberately e.g. for heat load control [11], introduce losses between the upstream and downstream locations. The validity of Eq. (2) due to this assumption has been examined in this work in order to provide guidance on its continued application. Furthermore, the legitimacy of the $T_{\text{e,sep}} \propto P_{\text{rad}}^2$ and $T_{\text{e,sep}} \propto P_{\text{rad}}^x$ scalings will be assessed in this paper.

2. Simulation set up

The edge fluid code EDGE2D [8] coupled to the kinetic neutral Monte-Carlo code EIRENE [9,10] was used to simulate a high confinement mode plasma in a set up as shown in reference [7] (high field side (HFS) and LFS strike points were located on the vertical target). The main fuel puff location was the same as used in reference [7]. However, the impurity puff location was moved to the LFS target in the private flux region so that it was in the same location as the experimental results presented in [11].

Simulations with two different seeding impurities – neon and nitrogen - were conducted. The impurities due to seeding were controlled within the simulation such that the total impurity seeding radiation achieved was either 2, 4 or 6 MW. For each seeded impurity and radiation power, a scan in upstream $n_{e,\text{sep}}$ was performed where the density was set to either 2, 2.5 or $3 \times 10^{19}$ m$^{-3}$. A total input power of 8 MW (split evenly between the ion and electron channel) was set as the core boundary condition for the heat flux into the domain. This parameter range was chosen to be representative of H-mode-like conditions for seeding scenarios [11]. The $3 \times 10^{19}$ m$^{-3}$, 6 MW, neon and nitrogen seeded simulations are not presented here due to code convergence issues. Unseeded reference cases were also simulated for each $n_{e,\text{sep}}$.

Beryllium was also included as a sputtered impurity from the main chamber wall in only the seeded simulations. Drifts and currents were not included within these simulations.

The radial transport in EDGE2D-EIRENE is diffusive only and pre-scribed. The radial particle and heat diffusion profiles were taken directly from references [12,13] for the main ions and electrons, and remained fixed throughout the presented parameter scan. Below the x-point the radial particle transport coefficients were set to 1 m$^2$s$^{-1}$ for the main ion and electrons. For the impurity ions it was assumed that the radial particle transport is poloidally and radially constant at 0.6 m$^2$s$^{-1}$ both above and below the x-point. The choice of the impurity transport coefficient is arbitrary, yet reasonable, due to having limited experimental knowledge about the radial transport of the impurity ions and aided in code convergence. The inclusion of a particle transport barrier in the radiating impurity was tested because a transport barrier was used in the main ions. At low, $n_{e,\text{sep}}$ $T_{\text{e,sep}}$ increased up to approximately 40%. However, the impurity transport barrier was found to produce very large core $Z_{\text{effective}}$ values, which were not experimentally relevant. At the highest $n_{e,\text{sep}}$ within this parameter scan, the transport barrier had minimal effect on $T_{\text{e,sep}}$ and $Z_{\text{effective}}$.

Details of the symbols used to represent the simulation on the proceeding figures are shown in Table 1.

3. Results

The purpose of this study was to compare the predicted $T_{\text{e,sep}}$ from EDGE2D-EIRENE with the prediction from Eq. (2). EDGE2D-EIRENE
Fig. 1. The upstream electron temperature calculated using the two point model equation $T_{u,sep} = \left(\frac{q_{P}}{\rho_{u}}\right)^{2}$ plotted against the EDGE2D temperature taken at the LFS midplane. The markers represent the total seeding radiation: circle – 0 MW (i.e. unseeded); triangle – 2 MW; square – 4 MW; 6-point star – 6 MW. The colour represents the seeding impurity: black – unseeded; green – nitrogen; blue – neon. Increasing size of the symbol represents increasing electron separatrix density ($n_{e,sep}$) where the smallest symbol is $n_{e,sep} = 2 \times 10^{19}$ and the largest is $n_{e,sep} = 3 \times 10^{20}$ m$^{-3}$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

was used as a synthetic experiment; parameters $P_{sep}$, $L$ and $A_q$ were extracted from EDGE2D to calculate Eq. (2) for a comparison with $T_{u,sep}$ predicted by EDGE2D-EIRENE.

3.1. Scaling of the upstream temperature with $q_1$ and $P_{sep}$

The derivation of Eq. (1) is based on the following assumptions: (1) the heat transport from the upstream to the downstream location is exclusively electron conduction (assuming it is much greater than the ion conductive heat flux) and calculated according to Spitzer–Härm [4]; (2) $T_{u,sep}$ is much greater than the downstream temperature i.e. $T_{D,sep}^2 \gg T_{u,sep}^2$; (3) $k$ remains constant along a field line; (4) $Lq_{|u,sep}$ captures the entire variation of the heat flux along the field line, i.e. $\int q_{u,sep}(s) \, ds \approx Lq_{|u,sep}$.

First, it must be established whether the assumptions stated in the previous paragraph can be validated within the presented parameter scan in order to proceed with a comparison of Eq. (2). Eq. (1) was calculated using the total $q_1$ at the divertor entrance at the separatrix ($q_{|u,sep}$). $L$ is calculated from the LFS target to the LFS midplane for all cases, and $k = 2000$ (Wm$^{-1}$eV$^{-2}$). Fig. 1 shows an agreement between the $T_{u,sep}$ measured in EDGE2D-EIRENE and the prediction from Eq. (1). Note the low density unseeded case (smallest black circle Fig. 1) is sheath limited, and when including the target temperature in Eq. (1) gives a better agreement with EDGE2D. The agreement was approximately within 20% at worst, and so a comparison with Eq. (2) was carried out.

The scaling $T_{u,sep} \propto q_{|u,sep}^{2}$ (as per Eq. (1)) for this simulation set, is valid due to all other variables in Eq. (1) (except $q_{|u,sep}$) being constant because the equilibrium remained fixed throughout the simulation set and $k$ remained approximately constant due to being a weak function of the plasma parameters. Approximately a factor six change in $q_{|u,sep}$ at the divertor entrance was observed (Fig. 2); hence the large variation in $q_{|u,sep}$ drives the two fold variation in $T_{u,sep}$. Based on the observation that $T_{u,sep} \propto q_{|u,sep}^{2}$ scaling is correct and $q_{|u,sep}$ varies by a factor six, it could be expected that $P_{sep}$ would also vary by a factor six ($q_{|u,sep} \propto P_{sep}^{\frac{1}{2}}$). However, a linear scaling between $T_{u,sep}$ and $P_{sep}$ was found (Fig. 3 solid markers), thus $P_{sep}$ only varies by approximately a factor two which would not support a factor two variation in $T_{u,sep}$. Hence, for the presented simulations, the scaling $T_{u,sep} \propto P_{sep}^{\frac{1}{2}}$ (solid lines Fig. 3) is not sufficient to explain the factor two variation in $T_{u,sep}$.

The scaling $T_{u,sep} \propto P_{sep}^{\frac{1}{2}}$, which assumes diffusive radial heat transport, is plotted for each $n_{e,sep}$ on Fig. 3 (dashed lines). For lower radiating cases, the scaling captures the variation in $T_{u,sep}$ to a reasonable degree. However, for higher radiating cases, greater than 4 MW for nitrogen and 2 MW for neon the scaling does not capture the variation in $T_{u,sep}$.

3.2. Variation in $P_{sep}$ is driven by core impurity radiation

A one-to-one correlation (within 1%) between the input power (into the grid) minus core impurity radiation and $P_{sep}$ was observed (Fig. 4). This implies that the observed variation in $P_{sep}$ is dictated by the amount of impurity radiation occurring inside the separatrix.

Comparing the radiative loss function [4] for a neon and nitrogen simulation with identical $n_{e,sep}$ and total impurity radiation, it was found that neon radiates more efficiently inside the separatrix than nitrogen [13]. Hence in all cases where $n_{e,sep}$ and the total impurity radiation was the same, neon had a lower $P_{sep}$ than nitrogen.

3.3. Variation in $q_{|u,sep}$ is partially driven by main SOL impurity radiation above the x-point

A reduction in $q_{|u,sep}$ was observed when the impurity radiation was present (Fig. 2). For a fixed $n_{e,sep}$ an increase in the total impurity radiation leads to a reduction in $q_{|u,sep}$ (Fig. 2). Furthermore, for a comparable simulation, similar $n_{e,sep}$ and total impurity radiation, neon seeding causes a larger reduction in $q_{|u,sep}$ than nitrogen compared to an unseeded simulation (Fig. 2).

To confirm that impurity radiation in the main SOL was an important mechanism for the variation in $q_{|u,sep}$, a code study was conducted. The code study removes the impurity radiation from the main SOL (above the x-point) only, but still allows for impurity radiation in the divertor (below the x-point) and core (inside the separatrix). Hence keeping $P_{sep}$ approximately the same. The impurity radiation was set to 2, 4 or 6 MW depending on the simulation chosen minus the contribution of the impurity radiation in the main SOL of that simulation. The radiation was set in this manner to ensure approximately the
symbols represent the same plasma parameters as the filled markers except within the simulation the impurity radiation has been removed from the scrape-off layer above the x-point. The dashed black line represents \( T_e = A P_{sep}^{2/3} \) where A was chosen to approximately intersect the unseeded simulation. The solid red line represents \( T_e = B P_{sep}^{2/3} \) where B was chosen to approximately intersect the unseeded simulation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. Input power (always 8 MW) to the computational domain minus the total impurity radiation within the separatrix versus the power crossing the separatrix. The markers represent the total seeding radiation: circle – 0 MW (i.e. unseeded); triangle – 2 MW; square – 4 MW; 6-point star – 6 MW. The colour represents the seeding impurity: black – unseeded; green – nitrogen; blue – neon. Increasing size of the symbol represents increasing electron separatrix density \( n_{e, sep} \) where the smallest symbol is \( n_{e, sep} = 2 \times 10^{19} \) and the largest is \( n_{e, sep} = 3 \times 10^{20} \). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 3. Upstream (LFS) electron temperature from EDGE2D versus power crossing the separatrix divided by 2 (assuming 50% split to HFS and LFS targets). Each plot represents a different separatrix electron density. The markers represent the total seeding radiation: circle – 0 MW (i.e. unseeded); triangle – 2 MW; square – 4 MW; 6-point star – 6 MW. The colour represents the seeding impurity: black – unseeded; green – nitrogen; blue – neon. Increasing size of the symbol represents increasing electron separatrix density \( n_{e, sep} \) where the smallest symbol is \( n_{e, sep} = 2 \times 10^{19} \) and the largest is \( n_{e, sep} = 3 \times 10^{20} \) m\(^{-3}\). The open square represents the seeding impurity: black – unseeded; green – nitrogen; blue – neon. Increasing size of the symbol represents increasing electron separatrix density \( n_{e, sep} \) where the smallest symbol is \( n_{e, sep} = 2 \times 10^{19} \) and the largest is \( n_{e, sep} = 3 \times 10^{20} \) m\(^{-3}\). For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

to calculate \( \lambda_{q, Eich} \) for each simulation. The choice to use the Eich fit is motivated by the fact that it is experimentally measurable, compared to directly measuring \( \lambda_q \) at the divertor entrance, which experimentally is impossible. Note that the 6 MW neon seeded case of \( n_{e, sep} = 2.5 \times 10^{19} \) m\(^{-3}\) did not have \( \lambda_{q, Eich} \) calculated because it was detached.

Using \( \lambda_{q, Eich} \) a value for \( A_q \) was calculated (as per Eq. (3)) which from now onwards will be referred to as \( A_{q, Eich} \). Extracting \( P_{sep, L} \) and \( B_{\theta}/B \) (note L and \( B_{\theta}/B \) are constant throughout the whole simulation set as the same equilibrium was used) from EDGE2D and using \( A_{q, Eich} \), an upstream temperature was calculated using Eq. (2). A comparison between this recalculated upstream temperature and the upstream temperature from EDGE2D is shown in Fig. 5. Agreement within approximately 20% of the predicted EDGE2D-EIRENE upstream temperature and the upstream temperature calculated from Eq. (2) was found (Fig. 5). Note that there is, at worst, a systematic underprediction of approximately 20% (Fig. 5) of the upstream temperature calculated from Eq. (2) when compared to EDGE2D. Accounting for the variation in both \( \lambda_{q, Eich} \) and \( P_{sep} \) in each simulation, agreement between Eq. (2) and EDGE2D was yielded.

Eq. (2) agrees with EDGE2D (Fig. 5) because \( (P_{sep}/2)/A_{q, Eich} \) scales with the variation in \( q_{||, u, sep} \) (Fig. 6). There is a large variation in \( A_{q, Eich} \).

3.4. Variation in Eich fitted \( \lambda_q \) captures the variation in \( q_{||, u, sep} \)

The total \( q_{||} \) profile at the LFS target was fitted using the Eich fit [14]
as \( \lambda_{q, \text{Eich}} \) varies by a factor four over the simulation set (vertical dashed lines Fig. 7). The simultaneous variation of both \( P_{\text{sep}} \) and \( A_{q, \text{Eich}} \) explains the variation in \( T_{\text{eu, sep}} \) in experimentally measurable variables. However, the reader should note that, no experimental evidence has been found to show that \( \lambda_{q, \text{Eich}} \) or \( \lambda_q \) scales with \( P_{\text{sep}} \).

The Eich fit is used to calculate \( \lambda_q \) because it correctly captures the variation in \( q_{||, u, \text{sep}} \). The radial variation in the \( q_{||} \) profile at the divertor entrance has changed from a typical exponential decay from the separatrix, and (3) a decrease in \( \lambda_q \) with increasing \( P_{\text{sep}} \) due to a balance of parallel and radial heat flux under the assumption of radially diffusive heat flux [4]. Simulations in which the impurity radiation in the main SOL was removed, the scaling \( T_{\text{eu, sep}} \propto P_{\text{sep}} \) captured the variation \( T_{\text{eu, sep}} \) of these simulations. This is because the scaling \( T_{\text{eu, sep}} \propto P_{\text{sep}} \) accounts for variation in \( P_{\text{sep}} \) and \( \lambda_q \) (assuming that is set by a competition between parallel heat conduction and prescribed diffusive radial heat transport).

Once the variation of \( q_{||, u, \text{sep}} \) was accounted for (by using experimentally derived variables \( P_{\text{sep}} \) and \( \lambda_{q, \text{Eich}} \)) an agreement within 20% between EDGE2D-FIRENE upstream temperature and the two point model equation (Eq. (2)) was yielded. A variation of upstream electron temperature from approximately 60–120 eV with seeding, for \( n_{u, \text{sep}} \) range of \( 2 \times 3 \times 10^{19} \) m\(^{-2} \), was observed. Hence it is incorrect to assume that the separatrix temperature is invariant due to the weak power scalings shown above. Models that are sensitive to the separatrix temperature should calculate \( \lambda_q \) and \( P_{\text{sep}} \) to predict \( T_{\text{eu, sep}} \) using the two point model equation.

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Supplementary materials


References

[3] H.R. Wilson, P.B. Snyder, G.T. a. Huysmans, R.L. Miller, Numerical studies of edge decay was captured well by the Eich fit.

4. Conclusion

An approximately two-fold increase in upstream temperature \( (T_{\text{eu, sep}}) \) was observed within EDGE2D, which is driven by a factor six change in the parallel heat flux entering the divertor at the separatrix \( (q_{||, u, \text{sep}}) \) thus confirming the scaling \( T_{\text{eu, sep}} \propto q_{||, u, \text{sep}} \frac{1}{2} \). However, only a factor two change in the power crossing the separatrix \( (P_{\text{sep}}) \) was observed. \( P_{\text{sep}} \) (for constant input power) is exclusively set by the impurity radiation occurring on closed field lines. \( P_{\text{sep}} \) was lower for neon seeded cases to a comparable nitrogen seeded case because neon radiates more efficiently on closed field lines than nitrogen, hence reducing \( P_{\text{sep}} \) and thus \( T_{\text{eu, sep}} \). The scaling \( T_{\text{eu, sep}} \propto q_{||, u, \text{sep}} \frac{1}{2} \) (which accounts for \( \lambda_q \) dependence on \( P_{\text{sep}} \) and for prescribed diffusive radial transport) captures the variation in the lower seeded simulation but not the higher seeded simulations. Variation in \( A_{q, \text{Eich}} \) (the perpendicular cross-sectional area of the considered flux tube) was strongly affected by the clipping of the near SOL \( q_{||} \) profile at the divertor entrance due to impurity radiation above the x-point, which renders the profile non-exponential. Nevertheless, our work shows that the Eich fit (which was used to calculate \( A_{q, \text{Eich}} \)) can still be used in conjunction with \( P_{\text{sep}} \) to approximate \( q_{||, u, \text{sep}}, T_{\text{eu, sep}} \) was driven by three things: (1) a factor two variation in \( P_{\text{sep}} \) due to varying core impurity radiation, (2) impurity radiation preferentially removing heat flux above the x-point and near the separatrix, and (3) a decrease in \( \lambda_q \) with increasing \( P_{\text{sep}} \) due to a balance of parallel and radial heat flux under the assumption of radially diffusive heat flux [4].


