

Critical Issues Identified by the Comparison between Experiment and SOLPS Modelling on ASDEX Upgrade

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Abstract. A detailed comparison between ASDEX Upgrade (AUG) experimental data and the results of SOLPS 2D edge code simulations revealed the tendency for the code solutions to underestimate the divertor electron temperature and overestimate its density. Extensive sensitivity studies of the SOLPS solutions to various assumptions in both plasma and neutral models were carried out in order to establish the cause of the discrepancies between the code and experiment. The possibility of an incorrect implementation of the neutral model in Eirene (the Monte-Carlo neutral part of SOLPS), or incorrectly described neutral balance in the divertor, has been almost ruled out. The most probable cause of the discrepancies is the presence of a significant population of supra-thermal electrons in the SOL and divertor plasma. They may, for example, increase parallel heat conduction in the divertor. It was established, however, that in order to obtain a ‘hot’ solution in the divertor, a rather significant increase, by factor > 4 , for the parallel electron heat conductivity $\chi_{e\parallel}$ is required. At the same time, an increase in the ion coefficient $\chi_{i\parallel}$ had very little impact on the divertor conditions.

SOLPS simulations also underestimate the magnitude of parallel ion flow in the SOL of AUG, confirming earlier experience of modelling JET flows with EDGE2D. It is likely that the two unresolved issues: failure of today’s 2D codes to model fast parallel ion flows in the SOL, and their underestimate of divertor T_e , are related to each other. There are indications from the SOLPS modelling that ‘hot’ divertor solutions with peaked target T_e profiles have positive radial electric field (E_r) in the SOL that increases the Pfirsch-Schlüter flow. In contrast, ‘cold’ divertor solutions are characterized by target T_e increasing with minor radius at the location of the maximum parallel ion flow, resulting in negative E_r that reduces the ion flow.

1. Introduction

SOLPS is a code package consisting of a fluid plasma code, B2, and a kinetic Monte-Carlo neutral solver, Eirene, for the plasma edge of tokamaks including outer core edge, scrape-off layer (SOL) and divertor regions [1-4]. It has been extensively used to model edge plasmas of ASDEX Upgrade (AUG) and some other existing machines (see e.g. [5,6]), as well as for predictions of divertor conditions in ITER (see e.g. [7]). For matched global parameters (mainly input power into the computational grid and radiated power) and matched upstream, midplane profiles, SOLPS reproduces experimental profiles and control parameters in the divertor with the accuracy within a factor of two [8,9]. However, recent detailed modelling of low density AUG H-mode [10] and medium density Ohmic [11] shots revealed the tendency for SOLPS solutions to underestimate the divertor electron temperature T_e and overestimate its density n_e . In case of the H-mode, the discrepancy between the experiment and the code solution was most pronounced near the outer strike point position, with the simulated peak H_α emission exceeding the measured signal by more than a factor of two. This feature is in qualitative agreement with earlier modelling of a JET H-mode shot with well-matched upstream parameters, where colder and denser plasma near the outer strike point than

measured in the experiment (by target Langmuir probes) was predicted by the EDGE2D code [12] (see FIG.1). For the AUG Ohmic shot, colder and denser plasma predicted by the code extended over the whole outer divertor.

Originally, two main possible causes of the discrepancies were considered: some

deficiencies in the neutral modelling (e.g. missing atomic and molecular reactions in Eirene, the Monte-Carlo neutral part of SOLPS), and the presence of a significant population of supra-thermal ions and

electrons in the SOL and divertor plasma. The results of dedicated SOLPS runs, where the sensitivity of the code solution to various assumptions of the neutral model was tested [10,11], strongly suggest that an incorrect neutral description cannot be the cause of the discrepancies. This is also confirmed by new sensitivity checks with varying neutral balance in the divertor by changing recycling, as described in Section 2. The working hypothesis currently is that the discrepancies are caused by supra-thermal electrons. In section 3, the possibility of a large increase in the parallel heat transport in the electron and ion channels is explored, leading to the conclusion that ‘hot’ (with high T_e) solutions in the divertor can be obtained when $\chi_{e\parallel}$ significantly exceeds its classical value. The influence of an increase in the ion coefficient, $\chi_{i\parallel}$, on the solution was found to be weak.

Alongside the new problem of discrepancies between the code and experiment in the divertor, there exists a long-standing issue of parallel ion flows in the SOL. The most thorough comparison between modelled (with EDGE2D) and experimentally measured flows (with the double-sided Langmuir probes, or ‘Mach probes’) was carried out on JET and showed that the code grossly underestimates the magnitude of the flows [13]. This conclusion is generally supported by the present modelling on AUG (with SOLPS). There are indications from the modelling, however, as shown in Section 4, that large Mach numbers of the parallel ion flow in the SOL can be obtained by the code for ‘hot’ divertor solutions. It is possible therefore that the two problems, of low predicted Mach numbers in the SOL and low target T_e , are related to each other, and both can be resolved provided ‘hot’ solutions can be obtained.

2. Influence of recycling on divertor parameters

As pointed out in the introduction, deficiencies of the neutral model in Eirene are no longer considered to be a probable explanation for the discrepancies in the divertor. A possibility was left open, however, for the particle balance in the divertor to be modelled incorrectly by assuming 100% recycling at the targets and walls, whereas in reality it may be $< 100\%$. The assumption of 100% recycling at the targets was justified on the grounds that the divertor

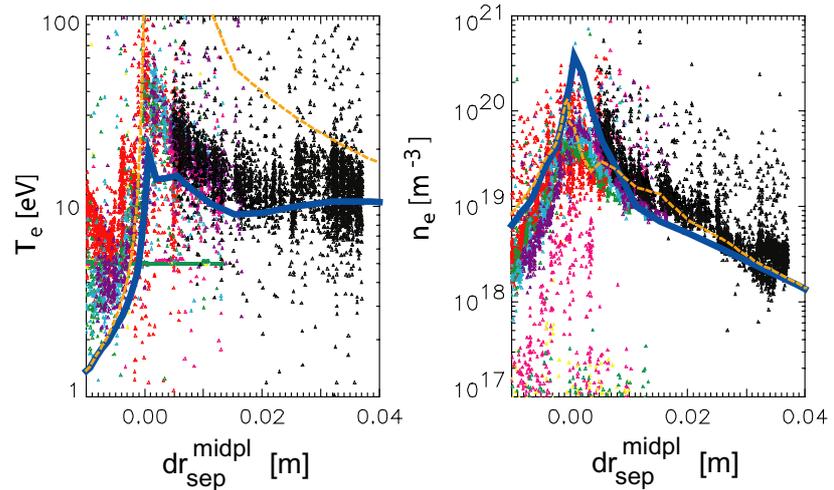


FIG.1. Langmuir probe measurements of electron temperature and density along the outer target obtained from a strike point sweep mapped to outer midplane coordinates. Data are compared to EDGE2D modelling (line) in between ELMs (thick blue line) and during an ELM (yellow dotted). Different colours of data points correspond to different probes. The lower boundary of the experimental data corresponds to inter-ELM phases. Figure replicated from ref. [12], with minor alterations.

target becomes saturated with deuterium on a rather short time scale. Nevertheless, it is still possible that, due to some residual pumping of some less saturated areas of the targets or the effect of the wall pumping, the effective removal rate of neutrals from the divertor in reality is higher than was assumed in the modelling, where the pumping was enacted mainly by the cryo-pump. This may reduce neutral pressure as well as plasma density in the divertor, leading to higher target T_e . To test the effect of such extra pumping, a series of SOLPS runs with the target recycling coefficient $< 100\%$ was made. As a continuation of the ‘sensitivity studies’ on the neutrals’ behaviour carried out earlier [10,11], the previously modelled AUG H-mode case with the separatrix density of $1.6 \times 10^{19} \text{ m}^{-3}$ and 3 MW of input power into the grid, without drifts, was used.

The results are presented in FIG.2. The target recycling coefficient was set to 0.9, 0.95, 0.97, 0.99 and 1. The following parameters were chosen to characterise SOLPS solutions: separatrix T_e at the outer midplane position (‘ T_e upstream sep.’), maximum T_e at the outer target (‘ T_e tar. max’), target T_e on the 1st ring outside of the separatrix, (‘ T_e tar. sep.’), ion flux through the innermost boundary of the numerical grid (‘Core flux’), and the ratio of peak values (simulated/experimental) of the H_α emission profiles at the outer target. It is clear from FIGs.2a,b, that a rather large reduction in the recycling coefficient, down to 0.9, is required in order to significantly raise the maximum target T_e . At this recycling coefficient, the H_α ratio is reduced to just below 1, which would be sufficient to match the experimental value for this

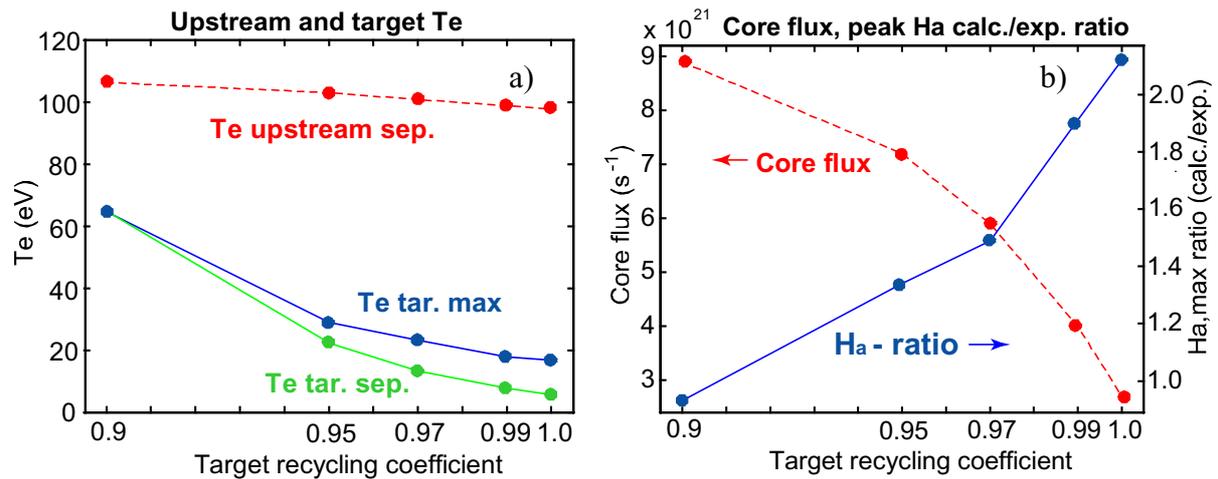


FIG.2. Upstream and target electron temperatures, a), particle flux through the innermost boundary of the grid, and ratio of peak values of H_α emission (simulated to experimental), b), in the series of SOLPS runs with variable target recycling coefficient. See text for details.

quantity. However, such a drastic reduction in the recycling coefficient sharply raises the neutrals’ pump-out and, subsequently, increases the ion radial flow through the inner core boundary of the SOLPS mesh by factor 3.3 compared with the reference case with 100% recycling, reaching $8.95 \times 10^{21} \text{ s}^{-1}$. This exceeds the sum of the ionisation source in the core region inside the grid ($4.43 \times 10^{21} \text{ s}^{-1}$) and the particle input from NBI ($4.8 \times 10^{21} \text{ s}^{-1}$) by factor 2, resulting in a gross violation of the particle balance. In other words, the number of neutrals originating at the target and walls and penetrating into the core, being ionised there and subsequently returned back to the SOL as ions, is far insufficient to maintain the combined inventory of ions and neutrals in the SOL and divertor regions due to the greatly increased pumping rate. Hence, such a high particle throughput must be considered unrealistic for the quasi-steady-state conditions modelled in [10]. Even for recycling coefficients ≈ 0.95 , there is a considerable mismatch in the particle balance. At the same time, for the coefficients above

0.95 SOLPS solutions don't predict changes in the target T_e and H_α profiles necessary for a match with the experiment.

3. Influence of the variation of parallel heat transport on divertor parameters

A large fraction of supra-thermal ions and electrons in the SOL can increase parallel heat flux conductivities compared to their classical values in the divertor. In particular, for the electron component, the application of 'flux limits' to parallel heat conductivity $\chi_{e\parallel}$ in divertor would be erroneous, and one should instead introduce 'flux enhancement factors', with $\chi_{e\parallel}$ exceeding its Spitzer-Härm value, as was concluded in the kinetic simulations in [14]. Nevertheless, upstream, the $\chi_{e\parallel}$ should indeed be limited, and the overall response of the plasma in the divertor is difficult to predict. As a way of assessing the potential impact of the $\chi_{e\parallel}$ rise, a series of SOLPS simulations were carried out where it was multiplied by constant factors f in the SOL and divertor regions. The results for the H-mode non-drift case described in the previous section are presented in FIG.3, for $f=1, 4$ and 10 . Both ion and electron flux limits were removed in these calculations. The upstream separatrix T_e at the outer midplane position dropped with the increase in f , in line with expectations, since for the same parallel heat flux $q_{e\parallel}$ it is related to f via $q_{e\parallel} \propto fT_{eu}^{7/2}$, provided the downstream, target T_e is much

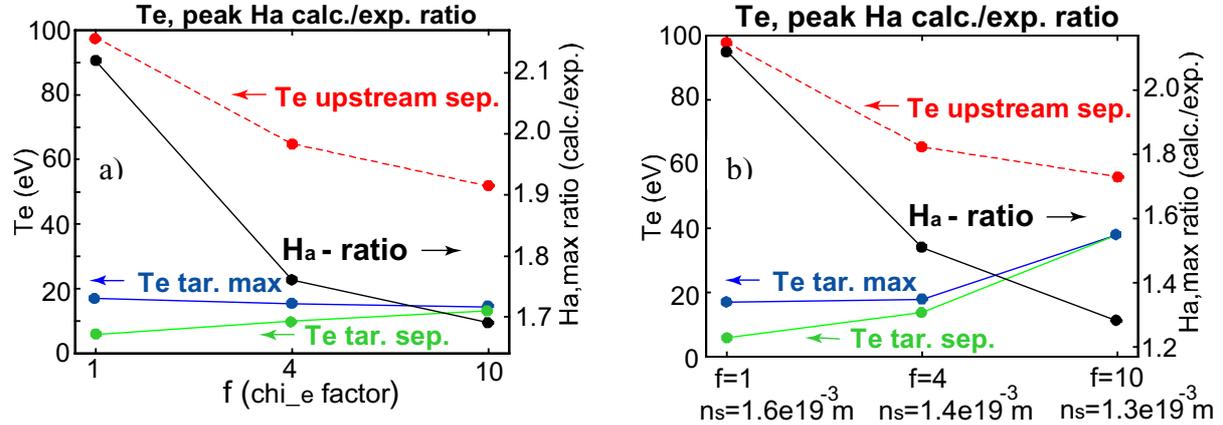


FIG.3. Upstream and target electron temperatures and the ratio of peak values of H_α emission (simulated to experimental), in the series of SOLPS runs with variable electron parallel heat flux enhancement factor f and separatrix density n_s . a) only factor f is varied, for constant $n_s=1.6e19$ m⁻³, b) both factor f and n_s are varied.

less than the upstream one: $T_{et} \ll T_{eu}$. The connection between the target and upstream T_e can be established by adding two other, very approximate relations: $n_u T_{eu} \propto n_t T_{et}$ (pressure

balance) and $q_{e\parallel} \propto q_t = \mathcal{M}_t T_{et}^{3/2}$ for the heat flux to the target, to yield: $T_{et} \propto \frac{T_{eu}^5}{n_{eu}^2} \left(\frac{f}{\gamma} \right)^2$, or

$T_{et} \propto \frac{q_{e\parallel}^{10/7}}{n_{eu}^2} \frac{f^{4/7}}{\gamma^2}$. As one can see from FIG.3a, the target T_e near the separatrix/strike point

position does indeed increase with f , however, due to 2D effects, the maximum target T_e is unchanged. The H_α ratio decreases, but remains substantially above 1. It is clear that raising factor f alone does not result in any appreciable increase in the target T_e nor in a sufficient reduction in the H_α radiation.

The reduction of the upstream T_e associated with the increase in $\chi_{e\parallel}$ (via factor f) allows one to also reduce the upstream n_e in SOLPS runs. Indeed, from experiment, one only obtains

pairs of T_e - n_e data points on the upstream profiles, since they come from the same laser diagnostic, while the exact location of the separatrix is poorly defined. FIG.3b presents the results of a series of runs where upstream separatrix n_e (n_s in the figure) is reduced, following the increase in f , keeping the separatrix T_e - n_e relation the same as in the experiment, with all other parameters, including input power, being unchanged. The strike point T_e now increases more steeply with f , while the maximum target T_e no longer drops. At $f=10$, the maximum in the target $T_e \approx 40$ eV, is reached at the strike point position, and the peak H_α ratio drops to 1.28, that is, the simulated peak H_α radiation is quite close to the measured value. The evolution of the target T_e profile is shown in FIG.4; it exhibits the progressive peaking of the profile with the increase in factor f . Summarising these modelling results, one concludes that rather high factors f , above 4, are required to achieve really ‘hot’ solutions in the divertor.

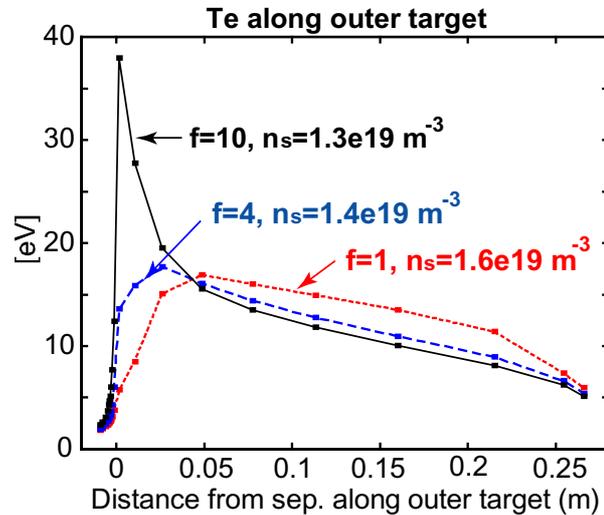


FIG.4. Electron temperature profiles at outer target for SOLPS cases with different factors f and separatrix density n_s .

Raising the ion coefficient, $\chi_{i||}$, (via the same factor f), on the contrary, did not result in any appreciable changes in the simulated target parameters. The ion component therefore is unlikely to be responsible for the discrepancies in the divertor.

4. Modelling parallel ion flow in the SOL

Measurements of the parallel ion flow on AUG in normal toroidal field (Bt) direction (ion ∇B drift directed towards the divertor) are described in [15]. They are in good qualitative agreement with earlier measurements in JET for the same magnetic configuration [13]. In both machines, the Mach number of the parallel ion flow reaches the peak value of ~ 0.5 some distance away from the separatrix (< 2 cm in JET and < 1 cm in AUG), and the flow is directed towards the inner divertor. The peak Mach number of the flow decreases at high plasma densities. In reversed Bt configuration (ion ∇B drift is away from the divertor) the Mach number is small in JET, while the peak value for the Mach number reverses its sign in AUG [16]. As was pointed out in [13], 2D code modelling usually predicts much lower absolute values of the parallel ion flow. This conclusion is generally confirmed by the SOLPS modelling.

For the AUG H-mode case modelled by SOLPS with drifts activated and described in [10], the parallel Mach number at the outer midplane did not exceed 0.15 (for the normal Bt case), which is much below typical experimental values for both Ohmic and H-mode plasmas [16]. At present, numerical instabilities in the core region of the computational mesh detrimentally affect SOLPS runs with drifts switched on, especially in cases with high core temperatures. In the present study, modelling with drifts was therefore confined to the lower temperature standard Ohmic AUG shot described in [11].

SOLPS radial profiles for the Mach number of the parallel ion flow across the outer midplane position are presented in FIG.5, for cases with the separatrix density $n_s = 1.3 \times 10^{19}$, 8×10^{18}

and $5 \times 10^{18} m^{-3}$, for normal and reversed Bt configurations. Out of these cases, only the normal Bt case with $n_s = 1.3 \times 10^{19} m^{-3}$ (shown in the top box) was matched to global plasma parameters and upstream profiles of AUG, as described in ref. [11]. The lower density cases, and all reversed Bt cases, have no experimental equivalents. The direction of the parallel flow corresponds to conventions adopted in SOLPS: namely, positive flow (Mach number) is directed from the inner to outer target. As can be seen from FIG.5, the profiles are not symmetric with respect to $M = 0$, and are affected by the plasma sink towards the outer divertor.

The difference between Mach numbers in normal and reversed Bt cases, ΔM , is indicated by arrows in FIG.5. The arrows are positioned at distances 0.5, 0.75 and 1.0 cm from the separatrix, roughly corresponding to the locations of maximum ΔM (ΔM_{\max}), but within 1.0 cm of the separatrix position, for the cases with the separatrix densities $n_s = 1.3 \times 10^{19} m^{-3}$, $8 \times 10^{18} m^{-3}$, and $5 \times 10^{18} m^{-3}$, respectively. The higher n_s case exhibits rather low Mach numbers, with $\Delta M_{\max} = 0.226$, which is significantly below typical measured Mach numbers for normal Bt configuration (~ 0.5). As the n_s is reduced, calculated ΔM_{\max} increases: to 0.326 and 0.474 for the two other cases.

Figure 6 shows a good match between the Mach numbers defined as $\Delta M_{\max}/2$, and those calculated using the Pfirsch-Schlüter formula for the

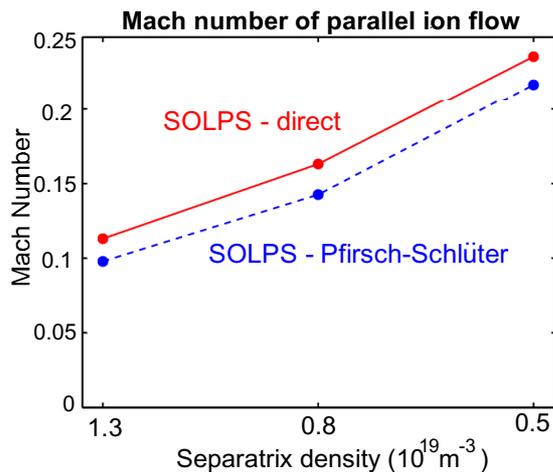


FIG.6. Mach number of parallel ion flow at positions indicated by arrows in FIG.5, directly obtained from SOLPS and calculated using the Pfirsch-Schlüter formula.

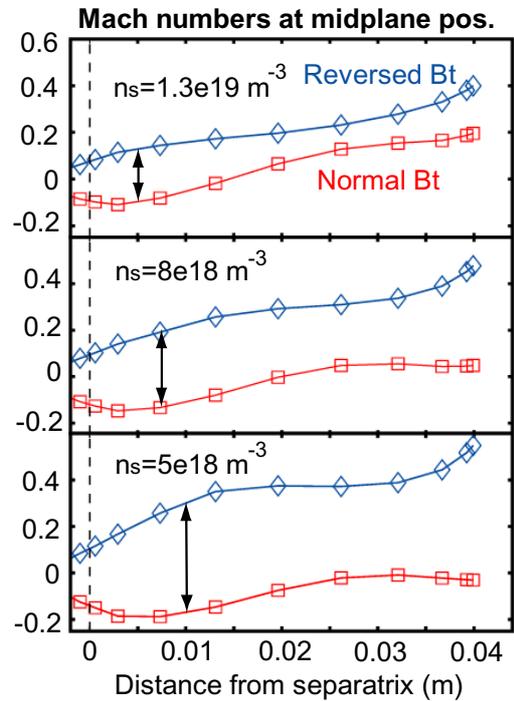


FIG.5. SOLPS calculated Mach number of parallel ion flow at outer midplane position, for 3 separatrix densities n_s and opposite toroidal field (Bt) directions.

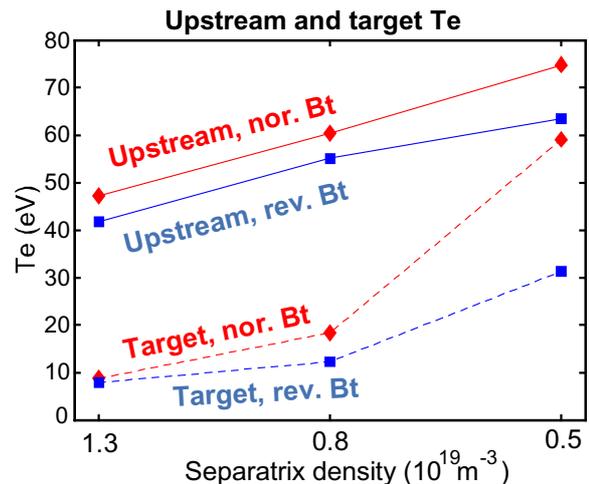


FIG.7. SOLPS modelled outer midplane and maximum target electron temperatures for cases with different separatrix density.

maximum parallel ion velocity: $V_{i\parallel, \max} = 2 \frac{a}{R} \frac{B}{B_\theta} \left(\frac{E_r}{B} - \frac{\nabla p_i}{B} \right)$, with the ion sound speed

defined as $c_s = \sqrt{(T_e + T_i)/m_i}$. Both Mach numbers increase with the decrease in the separatrix density. As n_s is decreased, both maximum target and midplane separatrix T_e increase (see FIG.7). About one half of the increase in the Mach number is due to changes in the decay length λ_{p_i} . The other half is attributed to changes in relative contribution of the E_r .

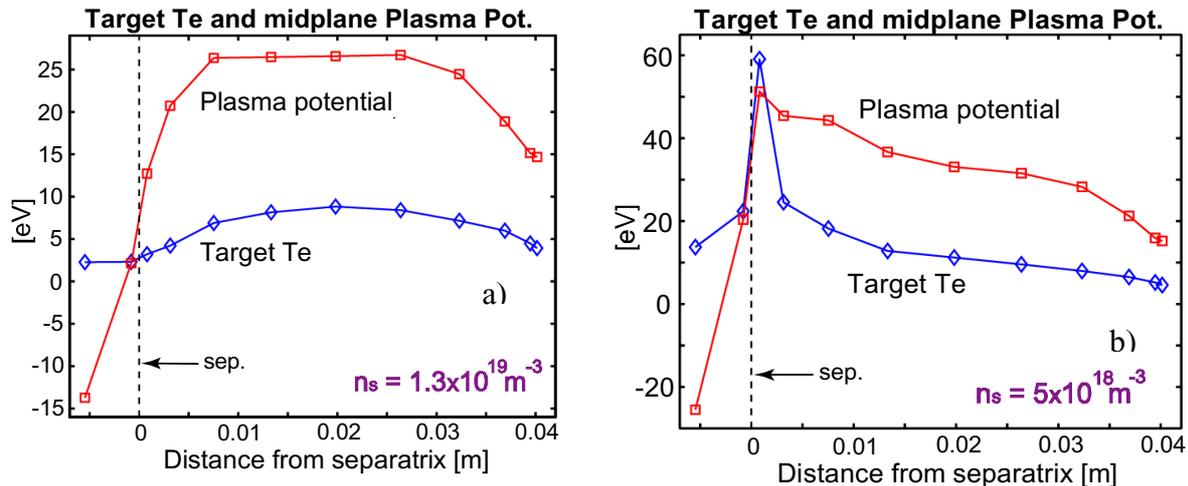


FIG.8. Outer target T_e mapped to outer midplane and outer midplane plasma potential profiles for normal Bt SOLPS cases and separatrix electron densities $n_s = 1.3 \times 10^{19} \text{ m}^{-3}$ (a) and $5 \times 10^{18} \text{ m}^{-3}$ (b).

For the highest n_s case, target T_e is low and increases with the minor radius, forming negative E_r at the position of the maximum Mach number due to the Debye sheath contribution. The contribution of E_r to the parallel plasma flow is therefore subtracted from that of the ∇p_i . At low n_s , the target T_e profile peaks near the strike point resulting in the formation of positive E_r that adds to the ∇p_i term. This is illustrated in FIGs.8a,b, where the outer target T_e and the plasma potential at the outer midplane are plotted for the cases with the highest and lowest n_s .

5. Summary

A detailed comparison between the ASDEX Upgrade (AUG) experimental data and SOLPS simulations was recently performed. High quality upstream profiles of electron density and ion and electron temperatures in the scrape-off layer (SOL) of AUG were collected for a low density ELMy H-mode shot and a medium density Ohmic shot. In both shots the tendency of SOLPS solutions to underestimate the divertor T_e and overestimate n_e was reliably established.

Extensive sensitivity studies of the SOLPS solutions were carried out. They revealed that the discrepancies between modelling and experiment are unlikely to be caused by deficiencies in the neutral modelling (e.g. missing atomic and molecular reactions in Eirene, the Monte-Carlo neutral part of SOLPS), or incorrectly described neutral balance in the divertor or the main chamber. More probable are explanations via the presence of a significant population of supra-thermal electrons in the divertor plasma. For typical plasma conditions in AUG, the bulk of the heat-carrying electrons upstream of the divertor (e.g., at the midplane position) are only weakly collisional, even for Ohmic plasmas. They may increase the effective parallel electron heat conductivity $\chi_{e\parallel}$ in the divertor compared to the classical Spitzer-Härm values.

SOLPS modelling with $\chi_{e\parallel}$ multiplied by various factors revealed that fairly large factors, > 4 , are required to transition the divertor from the ‘cold’ to the ‘hot’ solution. At the same time, increase in the *ion* parallel heat conduction coefficient did not result in any appreciable changes in divertor conditions. The ion component therefore is unlikely to be responsible for SOLPS failures to correctly predict divertor parameters.

In addition to discrepancies between modelled and experimental divertor conditions established in AUG, there exists a long-standing issue of discrepancies between modelled and experimental parallel ion flows in the SOL. It is possible that the two problems are related to each other. There are indications from the SOLPS modelling that ‘hot’ divertor conditions may be necessary for the formation of large parallel ion flows in the SOL. In the cases with high separatrix density, target T_e increases with minor radius at the position of the maximum parallel ion flow predicted by the code. The Debye sheath drop at the target then forms a negative E_r in the SOL reducing the contribution of the ion pressure gradient to the parallel Pfirsch-Schlüter flow. ‘Hot’ divertor solutions are presently realised in low density cases, with peaked T_e profiles, creating a positive E_r in the SOL that increases the ion flow.

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