Sensitivity of the boundary plasma to the plasma-material interface[1]

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Abstract

While the sensitivity of the scrape-off layer and divertor plasma to the highly uncertain cross-field transport assumptions is widely recognized, the plasma is also sensitive to the details of the plasma-material interface (PMI) models used as part of comprehensive predictive simulations. Here these PMI sensitivities are studied by varying the relevant sub-models within the SOLPS plasma transport code. Two aspects are explored: the sheath model used as a boundary condition in SOLPS, and fast particle reflection rates for ions impinging on a material surface. Both of these have been the study of recent high-fidelity simulation efforts aimed at improving the understanding and prediction of these phenomena. It is found that in both cases quantitative changes to the plasma solution result from modification of the PMI model, with a larger impact in the case of the reflection coefficient variation. This indicates the necessity to better quantify the uncertainties within the PMI models themselves, and perform thorough sensitivity analysis to propagate these throughout the boundary model; this is especially important for validation against experiment, where the error in the simulation is a critical and less-studied piece of the code-experiment comparison.

I. Introduction

The need for a predictive model for the boundary plasma has been widely recognized, given the challenges posed by the very high heat and particle fluxes and fluences expected in next-step devices including ITER [1]. Fluid models of the plasma transport in the scrape-off layer (SOL) and divertor, coupled to neutral transport simulations, are the current standard for predicting divertor operation in future experiments, with SOLPS [2], UEDGE [3], and EDGE2D-EIRENE [4] being the leading codes. These simulations are by necessity multi-physics, including models for plasma and neutral transport, atomic physics, and plasma-material interactions (PMI) such as the sheath very near material surfaces, erosion processes, and fuel recycling. The wide range of physics included in these fairly comprehensive models results in a complex, coupled system where errors have the potential to propagate in unexpected ways.

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Given the coupled nature of the problem, sensitivity analysis is a critical element of the overall verification and validation of the models as needed for confidence in predictive simulations. A major and well-known uncertainty in the model is that, lacking a physics-based model for cross-field plasma transport in the SOL, codes such as SOLPS and UEDGE simply assumed an ad-hoc value for the cross-field diffusivity [5] (occasionally with convective transport considered [6]). Uncertainties in the resulting SOL width has been a topic of vigorous experimental research recently [7,8,9,10], and sensitivity of predictions to these values have received attention from the modeling community as well [11]. However, uncertainty also exists in other aspects of the model beyond the cross-field transport, with effects and sensitivities that must be understood.

In this work we consider PMI-related uncertainties and their effect on SOL and divertor predictions using the SOLPS code. SOLPS assumes collisional transport parallel to the magnetic field (with some kinetic corrections) and user-specified cross-field transport. Neutral transport is calculated using the Monte Carlo code EIRENE [12], and an extensive set of atomic physics rates and PMI processes are included via databases. For these studies SOLPS version 5.0 is used, with the 1999 version of EIRENE. Further details of the overall model can be found in Ref [13]. Two specific PMI features are studied here: the impact of the sheath characteristics that are set as boundary conditions on the plasma fluid equations, and the impact of large changes to the particle and energy reflection coefficients for ions and neutrals striking material surfaces. Improving models for both the sheath and surface reflection have been the focus of recent full-physics simulation efforts, as described in more detail below. Part of the purpose of the present work is to study the overall impact that these improvements have on the plasma solution. However, a second and more long-term goal is to begin the process of sensitivity analysis needed for rigorous uncertainty quantification and validation. While no direct comparisons to experiment are made here, a major goal of this line of research is to validate models against experimental data. Performing a rigorous error analysis on the simulations, including the effects of PMI-related uncertainties as studies here, is a necessary part of making comparisons to experiments for the purposes of validation.

II. Sheath heat transmission

The so-called plasma sheath that forms at the interface between a plasma and a material surface plays a critical role in regulating the plasma heat and particle flow to the surface [14]. It effectively determines the plasma flow speed and heat flux given parameters of the plasma impinging on a surface, as described in more detail in a companion paper [15]. Since the sheath region is typically physically small, being on the scale of as low as μm depending on plasma conditions, it is typically treated simply as a boundary condition on the plasma fluid equations that are solved in codes such as SOLPS. For the plasma flow speed, the Bohm condition that the parallel ion speed is at least the sound speed c_s is applied:

$$v_{\parallel} \geq c_s \equiv \sqrt{\frac{k\left(T_e + T_i\right)}{m_i}} \tag{1}$$

Where k is the Boltzmann factor, T_e and T_i are the electron and ion temperatures, respectively, and m_i is the ion mass. For the electron and ion heat fluxes, the following boundary conditions are applied at the sheath entrance:

$$q_{i,e} = \gamma_{i,e} \Gamma T_{i,e} \tag{2}$$

Where Γ is the ambipolar particle flux consistent with the Bohm condition above ($\Gamma = nc_s$) and $\gamma_{i,e}$ are the sheath heat transmission factors for the ions and electrons. These sheath transmission factors are calculated based on kinetic models, with typical values of γ_i~1.5-2.5 and γ_e~4.5 used in fluid modeling [16].

Recent full-physics particle-in-cell kinetic simulations using the VPIC code [17] have resulted in improved calculations of the factors described above setting the sheath boundary conditions on the fluid plasma calculations [18]. These calculations show fairly standard values for the electron sheath heat transmission factor, in the range of 4-5 depending on collisionality. However, the transmission factor for the ions is much higher than is typically assumed, being γ_i~5.5 for the cases considered [18]. This value of more than double the standard assumptions in

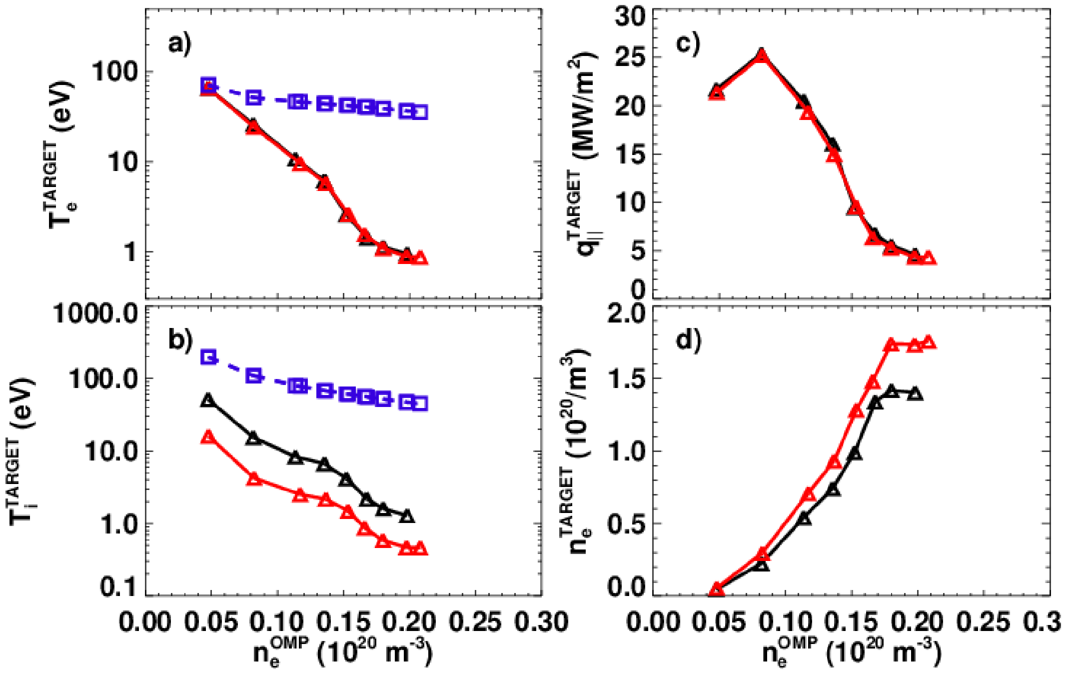

Figure 1: Variation of a) electron temperature, b) ion temperature, c) parallel heat flux and d) electron density at the outer divertor as midplane density is varied. Simulations using standard sheath transmission factors are shown in black, those using values indicated by VPIC in red; the temperature at the outer midplane is indicated by blue squares.

fluid modeling has the potential to substantially alter the resulting equilibrium transport solution away from that produced using a standard sheath model.

The impact of this new factor γ_i based on full-physics kinetic simulation has been tested in a set of SOLPS calculations. The grid for these calculations is based on a magnetic equilibrium with major radius R=1.7 m, aspect ratio R/a~3, elongation κ~1.7, and δ~0.2; this is based on the analysis described in more detail in Ref [13]. The assumptions used in the modeling are not based on any measurements or specific experiments, but are chosen to facilitate straightforward analysis of the various sensitivities. All charge states of deuterium and carbon are included in the simulations, with carbon being introduced via physical and chemical sputtering the walls. The cross-field transport coefficients are held constant throughout this work at D=0.25 and $\chi_e=\chi_i=1.0$ m^2/s. These produce a heat flux width in the SOL of λ_q~0.5-1.0 cm. A total power of 1 MW is input into the simulation, evenly shared between electrons and ions; overall these parameters are roughly consistent with L-mode experiments (although again no attempt is made to reproduce a particular experimental condition).

Figure 1 shows the results of a simulated density scan, using both the standard values for the sheath heat transmission coefficients (γ_e=4.5, γ_i=2.5), and using the updated VPIC values

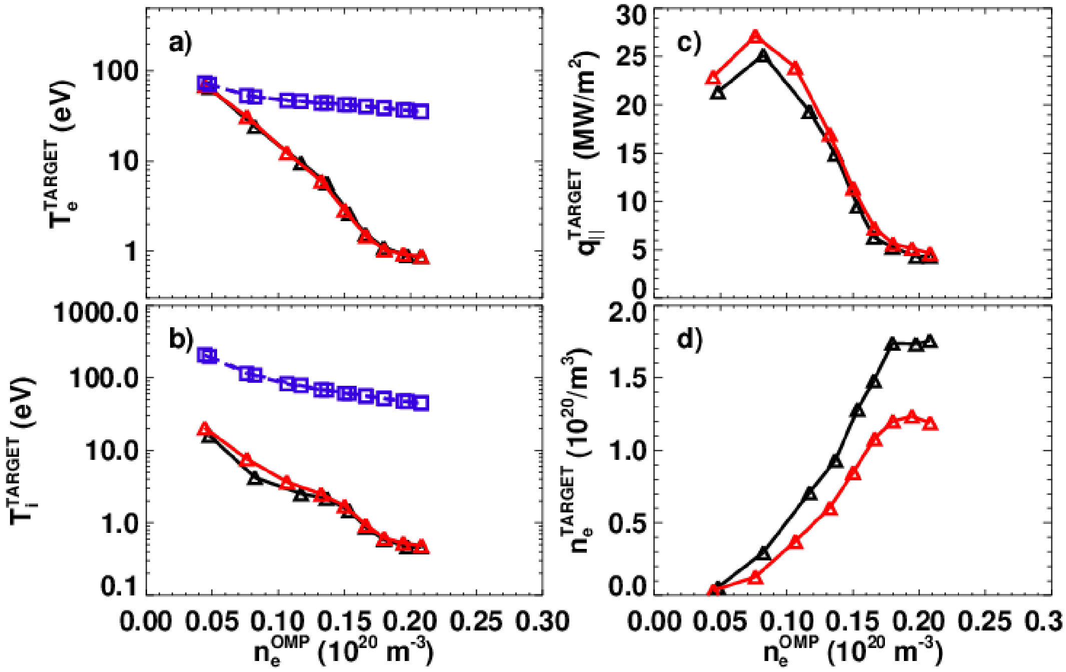

Figure 2: Variation of a) electron temperature, b) ion temperature, c) parallel heat flux and d) electron density at the outer divertor as midplane density is varied. Simulations using standard sheath flow speed boundary in black, those using values indicated by VPIC in red; the temperature at the outer midplane is indicated by blue squares.

(γ_e=4.5, γ_i=5.5). The quantities are shown are taken at end of a flux tube located ~1mm radially from the separatrix at the outer midplane, showing parameters at the surface of the outer divertor plate. These are shown as a function of midplane density on that same flux tube, since the two-point model for the SOL shows a strong dependence of divertor parameters on the upstream density [16]. Perhaps not surprisingly, the largest impact is on the ion temperature, which shows substantially lower T_i with the VPIC sheath model. This is consistent with higher heat transmission resulting in reduced ion temperature needed to exhaust the same power (i.e., to keep the quantity $\gamma_i T_i \Gamma$ constant). The electron density shows a modest increase with the VPIC model, partially offsetting the impact of the reduced ion temperature on the total pressure. The electron temperature and parallel heat flux are essentially unchanged between the standard and VPIC model, as is the particle flux (not shown). This indicates that the overall power and particle balance is not directly affected by the modified sheath model, but instead the ion temperature adjusts to keep the heat through the sheath constant. Since T_e plays a stronger role in setting the various atomic physics rates (aside from charge exchange), the overall impact on the plasma solution is fairly modest. One critical prediction of simulations such as these is determining the upstream density at which a low-T_e, low-$q_{||}$ and hence highly dissipative regime can be accessed. This in part determines the operation conditions that are required to ensure sufficiently low net erosion and heat flux control [19]. Thus an important feature of the comparison of sheath transmission factors is that access to the low-T_e, low-q|| regime is unchanged in terms of the upstream density requirements. This implies that the update to the sheath model studies here will not have a large impact on the operating regime for future devices (at least based on the cases studied here).

A second result from the VPIC simulations is a deviation in the standard assumption for the flow speed: unlike the expression given in Eq. 1, VPIC indicates that an ion adiabatic factor of 3 is more appropriate, so that

$$v_{\|} \geq c_s \equiv \sqrt{\frac{k\left(T_e + 3T_i\right)}{m_i}} \tag{3}$$

Further, the VPIC calculations indicate that the plasma flow is substantially super-sonic for all collisionalities considered, with a mach number (using the definition of the sound speed given in Eq. 2) $M=v_{||}/c_s$=1.1-1.3. The impact of this change to the flow speed has also been tested in SOLPS, by setting the mach number at the boundary to

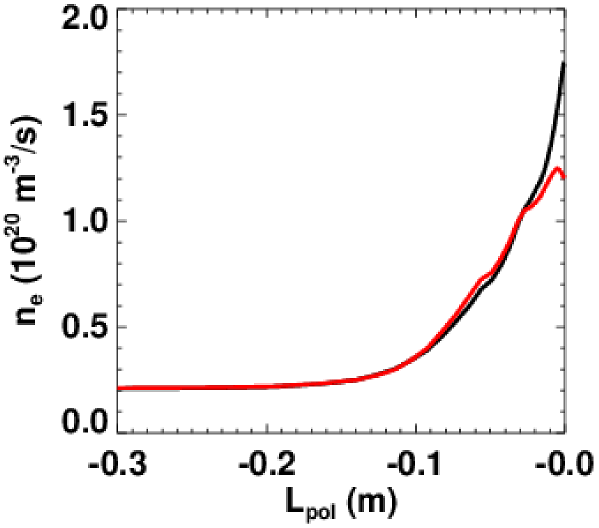

Figure 3: Poloidal profiles along the 1mm flux tube of the electron density for the standard flow boundary condition (black), and using M=1.5 (red). L_{pol}=0 corresponds to the outer target plate.

1.5 (using the sound speed in Eq 1). For T_e=T_i, this is equivalent to the VPIC definition of the mach number with M~1.1, consistent with the results presented in Ref [18]. The results of this test are shown in Figure 2. In this case the largest change is to the electron density at the target, which decreases by ~30%. A modest increase in the ion temperature is observed, and slightly higher parallel heat flux such that higher upstream density is required to reach the same parallel heat flux with the higher flow speed boundary condition.

It is somewhat counterintuitive that the change to the parallel heat flux should be so small, since the large change to the electron density should in principle carry over to a modification of the radiation profile and hence power balance. However, the change in the electron density with the VPIC-based mach condition occurs only over the thin region near the surface where recycling is strong and flow transitions from low values to sonic, as shown in Figure 3; over the bulk of the SOL and divertor, the density is essentially the same for the two cases. Since volumetric power loss occurs throughout the divertor volume, the impact on radiated losses of this narrow region with suppressed density is modest. However, this may not be universal: in next-step, very high power devices, modeling often predict radiation patterns that are also quite localized near the target [20]. In such a case, reducing the density over the same region could have a substanatial impact on the radiative power dispersal.

III. Energy reflection

A second set of sensitivity studies have also been performed, testing the role of direct reflection of particles and energy incident on the material surface. This is motivated by recent molecular dynamics calculations for He incident on W (highly relevant to the He phase of ITER operation), which show very high reflection coefficients [21]. For more highly-studied low-Z wall systems such as deuterium incident on carbon, typical reflection coefficients are fairly low, with values for reflection $R_{N,E}$~0.3 as calculated by standard codes such as TRIM [22] (this represents the fraction of incident particles that undergo direct reflection; the rest are usually assumed to recycle as atoms or molecules at the temperature of the wall). The new MD data indicates R_f that can approach unity (depending on the incident angle and energy), significantly higher than that indicated by standard binary collision approximation codes such as SRIM [21].

The impact of high reflection has been tested using the same SOLPS base case as described in the section above. Although the high values for $R_{N,E}$ presented in Ref [21] are for helium ions impacting on tungsten, here we maintain the plasma and wall composition as deuterium and carbon, respectively, and artificially increase the values of $R_{N,E}$ towards those indicated in [21]. This is done to minimize the number of simultaneous changes to the simulation and thereby simplify the interpretation, allowing the impact of $R_{N,E}$ to be isolated. As such, these calculations are only indicative, and not directly comparable to what might be expected to occur in experiment when transitioning from a low-reflection system (D->C) to high (He->W). It should be noted that the change in particle and energy reflection due to different plasma and wall composition is already accounted for within SOLPS calculations for, e.g., ITER, and has been studied to a degree as part of the changeover of the JET tokamak to an ITER-like metal wall [23]. The new aspect in the present work is the additionally higher reflection coefficients studies, based on the new MD calculations which indicated significantly higher values than previously obtained [21].

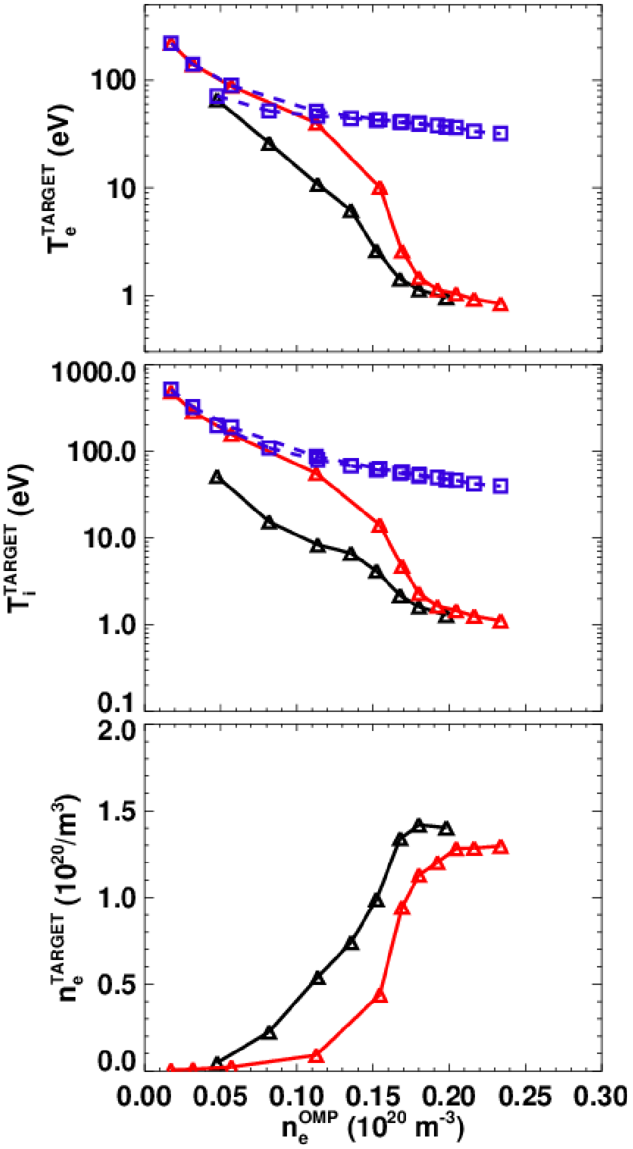

Figure 4: Variation of a) electron temperature, b) ion temperature, c) electron density at the outer divertor as midplane density is varied. Simulations using TRIM-calculated values for reflection for D on C are shown in black, those using Rf=0.75 in red.

The impact of increasing R_f from the TRIM values for deuterium on carbon to 0.75 (more representative of He on W) on the calculated plasma solution is shown in Figure 4. The largest change compared to the low-reflection case is in the plasma temperatures, which increases substantially for both electrons and ions (with T_i increasing more strongly). This is intuitively unsurprising, as the reduction in net power to the wall when a large fraction is reflected suggests that a hotter plasma is required to produce the same net heat exhaust. The increase in T_e and T_i is more marked at low plasma density; at the highest densities the plasma is less strongly impacted, and the low T_e regime required for power dissipation and erosion control is still accessible. However, the access to this low-T_e regime is significantly affected by these changes to reflection, with approximately 20% higher upstream density required to reduce T_e below 5 eV in the high-reflection case. This indicates that the ion reflection properties of the surface material can have a substantial quantitative impact in determining plasma operating conditions compatible with long PFC lifetimes. Further studies more targeted at a helium plasma impinging on either carbon or tungsten are warranted and will be pursued as part of future research.

IV. Discussion and conclusions

The sensitivity of the plasma solution as calculated by the SOLPS fluid code to two PMI-related characteristics has been studies: the plasma sheath parameters set as boundary conditions to the fluid equations, and the fast particle reflection coefficient associated with ions striking material surfaces. These changes to the SOLPS model are based on recent studies where high-performance simulations were used to increase the physics fidelity of the specific models. In all cases the changes to the models resulted in quantitative changes to the plasma solution. The updated sheath ion heat transmission coefficient, based on improved full-physics PIC simulation, had the strongest impact on the ion temperature, with a weaker effect on the electron density and little impact on the heat and particle fluxes. The high flow speeds indicated by the same PIC simulation had the effect of reducing the density at the wall, but again little impact on the fluxes. Raising the fast particle reflection coefficient had a more dramatic impact on the plasma solution, significantly increasing both T_e and T_i, especially at low densities.

In all cases the plasma solutions are qualitatively similar to the standard set of assumptions, in that at sufficiently high upstream density a low temperature divertor regime with strong power dissipation can be accessed. The upstream density required to reach these conditions is modestly impacted by the parameters varied here for the most part, with the largest change being ~20% in the high-reflection case. These results suggest that the impact of the PMI-related uncertainties studied here will not have a profound impact on the operating regime of the divertor of large future devices, although the divertor conditions at a given upstream density can be strongly altered. However, the larger purpose of this study is to begin a sensitivity analysis as needed as a part of uncertainty quantification. This is a necessary part of the validation process, which is urgently needed for plasma boundary models in order to gain confidence in their predictive capability. The quantitative dependences of the plasma on the PMI parameters studies here will need to be taken into account in validation studies, especially true at lower densities that are not in the dissipative divertor regime (and at which current experiments often operate). Performing these studies including comparisons to experiment will be a part of future research. A final conclusion that may be drawn from this study is that, at least for the cases studied here, the plasma solution appears to be less sensitive to the sheath transmission characteristics than to the surface interactions, suggesting that improving surface models may the more urgent research areas

Acknowledgements

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