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Testing the role of molecular physics in dissipative divertor operations through helium plasmas at DIII-D

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Recent experiments in DIII-D helium plasmas are examined to resolve the role of atomic and molecular physics in major discrepancies between experiment and modeling of dissipative divertor operation. Helium operation removes the complicated molecular processes of deuterium plasmas that are a prime candidate for the inability of standard fluid models to reproduce dissipative divertor operation, primarily the consistent under-prediction of radiated power. Modeling of these experiments shows that the full divertor radiation can be accounted for, but only if measures are taken to ensure that the model reproduces the measured divertor density. Relying on upstream measurements instead results in a lower divertor density and radiation than is measured, indicating a need for improved modeling of the connection between the divertor and the upstream scrape-off layer. These results show that fluid models are able to quantitatively describe the divertor-region plasma, including radiative losses, and indicate that efforts to improve the fidelity of the molecular deuterium models are likely to help resolve the discrepancy in radiation for deuterium plasmas. Published by AIP Publishing.

4Invited speaker.]
inadequacies in many parts of the physics basis could contribute to the radiation deficit. Hence, the underlying source of radiation shortfall may be something other than the deuterium atomic and molecular physics completeness and accuracy, and improving on these will not fully resolve the discrepancy if the true issue is a more fundamental inadequacy of the 2D fluid plasma model in describing SOL and divertor physics. Indeed, it is well-known that this model neglects or incompletely treats many important physics features that are thought to be important elements in describing the boundary plasma (e.g., kinetic effects and turbulence).

In the present work, we describe a set of experiments and modeling activities aimed at testing the possibility whether the atomic and molecular physics basis is indeed the likely underlying inadequacy responsible for the observed radiation deficit. These made use of helium plasmas designed to test radiative divertor operation. Operating in helium has the advantage of simply removing the complicated molecular processes under suspicion from the scenario, indirectly allowing their contribution to radiation shortfall to be assessed. Helium operation also removes chemical sputtering of carbon, largely eliminating carbon radiation at low divertor temperatures where physical sputtering yields are also small. Hence, the simple presence or absence of a radiation deficit in helium plasmas should offer insight into the possible sources of error in the model. The analysis described here also explores the possible role of transport physics and how the measured density is matched in modeling and attempts to isolate these effects from atomic physics on radiation levels. Overall, this work aims to inform the likelihood that whether better capturing the complicated molecular physics in deuterium will improve the overall agreement with experiment.

II. SETUP OF EXPERIMENTS AND CORRESPONDING MODELING

The radiated power density \( P_{\text{rad}} \) can be written as

\[
P_{\text{rad}} = n_e n_Z L_Z(T_e, n_e \tau),
\]

where \( n_e \) and \( n_Z \) are the electron and impurity densities, respectively, \( L_Z \) is the radiation power function which is determined by atomic physics and the charge state distribution of the plasma which in turns depends on the electron temperature \( T_e \) and the impurity transport through the replacement time \( \tau \). Already, this illustrates the range of possible sources of error in the calculation of radiation, as it depends on the background plasma \((n_e, T_e)\), impurity generation and transport physics \((n_Z, \tau)\), and atomic physics \((L_Z)\).

Studies of radiative divertor operation in helium plasmas have been performed due to the potential to simplify the set of physical processes involved and hence perform a more fundamental test of models’ ability to capture radiation physics. Since helium plasmas do not involve molecular processes, the set of atomic reactions that could contribute to \( L_Z \) are limited and are able to be treated more completely. The atomic physics rates may themselves not be necessarily more accurate than those for deuterium, but they can be included more comprehensively. Furthermore, the lack of chemical erosion removes carbon as a strong radiator at low divertor temperatures, so that the source and density of the radiator are less uncertain. By testing the ability of the models to capture radiation in this simplified environment, we can evaluate whether improving the atomic and molecular physics included in modeling deuterium plasmas is likely to resolve the radiation discrepancy, or whether it is caused by other physics missing from the models.

The experiments were performed on the DIII-D tokamak.\(^{15}\) The general plasma characteristics are similar to experiments described elsewhere that have been optimized for divertor diagnosis.\(^{16}\) The neutral beams used to heat the discharges were converted to helium operation, so that strong heating could be performed while maintaining high purity of the helium plasma. The injected beam power in the discharges studied here was 2 MW, for a total power (including Ohmic heating) of \( \sim 3–3.2 \) MW. The plasmas described here remained in the L-mode throughout the time periods of interest. The outer strike point position was varied on a shot-by-shot basis (i.e., shots were repeated at varying strike point locations) in order to build a 2D map of electron density \((n_e)\) and temperature \((T_e)\) measurements using the Divertor Thomson Scattering (DTS) system.\(^{16}\) The density was ramped during each shot, as illustrated in the time traces shown in Figure 1; the shot numbers in consideration are 166819-826. The range of density sweep spanned the divertor regimes of interest, from strongly attached at low density up to strongly detached with high radiated power at high density. Data are combined from different discharges to produce the 2D \( n_e \) and \( T_e \) maps. Data with line-averaged density within 5% of that at the center of the time window were included. The strike point position was only varied over...
a limited range such that the outer divertor volume was probed; data from the inner divertor leg are not available from these discharges using the DTS system. The other primary diagnostics used in this work include upstream density and temperature measurements using Thomson scattering and charge exchange recombination spectroscopy and measurements of the 2D radiated power distribution from tomographic inversions of bolometric measurements.

Modeling of these experiments has been performed using the SOLPS (Scrape-Off Layer Plasma Simulation) suite of codes. This uses a 2D fluid model for the plasma transport via the B2.5 code, which is coupled to a Monte Carlo calculation of the kinetic neutral transport using the EIRENE code (in the present work, the 1999 version of EIRENE is used). Plasma transport is assumed to be classical in the direction parallel to magnetic field lines, with kinetic corrections implanted by flux limiters on the electron and ion heat flux, as well as the parallel viscosity. Transport across magnetic flux surfaces is governed by user-specified cross-field transport coefficients \( D, \chi_e, \) and \( \chi_i. \) The plasma sheath at the intersection between plasma and material surfaces is implemented via boundary conditions on the fluid equations, with standard values for the sheath heat transmission coefficients and sonic parallel flow \( v_{||} = \frac{v_{i}}{c_s} = 1, \) where \( c_s \) is the sound speed) assumed. Physical and chemical sputtering of the PFCs by ion impact is included using standard databases, and atomic reactions for ionization, recombination, and charge exchange are included using rates as in Ref. 19. It should be noted that \( E \times B \) and diamagnetic drifts are not included in the present work due to associated numerical difficulties. This makes the present effort unlikely to capture the in-out divertor asymmetries that have been previously measured and modeled, as these are known to be impacted by drifts. However, the impact of drifts on the radiation levels has been previously shown to be modest (~10%), and further drifts are expected to be less important at the low divertor temperatures of most interest for dissipative divertor analysis. In any case, the present work focuses on the outer divertor due to both the available measurements and this limitation in the modeling.

In principle, the cross-field transport coefficients representing anomalous diffusion should be taken from a physics-based transport model in order for the overall edge plasma model to be truly predictive. However, as reliable SOL transport models are lacking (although they are currently an active area of research), experimental measurements are instead used to constrain the SOLPS modeling. This is accomplished by adjusting the transport coefficients using an iterative procedure until a good match to the measured \( n_e \) and \( T_e, \) upstream profiles is produced. While in principle the same method can be used to reproduce the \( T_i \) profile, in practice ion measurements in the SOL are typically sparse and difficult to interpret when available; instead, a typical value for the ion heat diffusivity (1 m/s) is used. This procedure effectively allows the upstream electron profiles to be set as input into the SOLPS modeling; while a fairly standard method for analysis of experiments using edge transport codes, this has important implications which will be discussed below.

### III. COMPARISON OF RADIATION CHARACTERISTICS WITH MATCHED UPSTREAM PROFILES

Three time slices from the helium discharges have been modeled using the above method, as indicated by the vertical lines in Figure 1. These times span from an attached divertor with high temperature \( (T_{e, \text{div}} \sim 15 \text{ eV}) \) and modest radiation to a highly radiating, low-temperature \( (T_{e, \text{div}} \sim 2 \text{ eV}) \) high density \( (n_{e, \text{div}} \sim 3 \times 10^{20} \text{ m}^{-3}) \) case. 2D profiles of the divertor radiation are shown in Figure 2, based on bolometric inversions. At the lowest density, the radiation in the outer divertor is localized near the surface of the PFC, and as the density is increased, the radiation zone moves upwards towards the X-point. However, at the highest density considered, the radiation is still dominantly from within the divertor region. This is noteworthy, as previous helium detachment experiments have shown that radiation often collapses to the X-point, leading to little power flowing into the SOL and divertor itself; this scenario is less interesting from the standpoint of studying a dissipative divertor. In the present experiments, the power flowing into the SOL remains high and is dissipated within the divertor volume; this combined with the achievement of a high-recycling SOL regime (evidenced by the high divertor densities) makes the present study more relevant to testing the ability of models to reproduce dissipative divertor physics. Times later in the discharges show strong X-point radiation and are hence excluded from the present analysis. While not shown here,
carbon is effectively removed from the two high density time slices (due to a lack of chemical sputtering), with very little visible carbon emission measured compared either to the earlier time point (where physical sputtering is higher) or to similar deuterium plasmas.

The upstream profiles resulting from the fitting technique described above are shown in Figure 3 for the lowest-density time slice ($t = 1600$ ms). As can be seen, the profiles are well-reproduced by SOLPS (the quality of the fit is similar for the other two time points). In all calculations, the experimental power into the SOL ($\sim 3$ MW) is set as a boundary condition, but the power flux to the target is not directly constrained in the modeling. The SOLPS-calculated radiated power distributions are shown in Figure 4 and show good qualitative agreement with measurements: the radiation is localized near the target at low density and moves towards but not all the way to the X-point at the highest density modeled. However, the magnitude of the total radiation integrated over the outer divertor is consistently lower from SOLPS modeling than the measured value as shown in Figure 5, which shows the radiation from experiment and from modeling as a function of the upstream separatrix density. This is similar to the case in deuterium as described above, although the discrepancy is lower in magnitude (with SOLPS being only $\sim 25\%$–$35\%$ lower than experiment at high densities, in comparison to a factor of $\sim 2$ reported for deuterium). Thus, while the radiation deficit is reduced in helium, for matched upstream plasma profiles a substantial radiation shortfall remains.

A possible source of this radiation deficit has been identified from comparisons of the divertor profiles between modeling and experiment. With the upstream profiles used as a constraint on the modeling, the reproduction of the divertor plasma characteristics is not guaranteed. Fortunately, DIII-D has the unique capability of directly measuring $n_e$ and $T_e$ within the divertor volume based on Thomson scattering as described above. The measured and modeled density distributions for the lowest-density time slices are shown in Figure 6 and show a consistently lower density in the SOLPS modeling than is measured by DTS. The full 2D profiles in the outer divertor are shown (panels a and b), as well as a 1-D profile of the same data plotted along a flux tube very near the separatrix. The discrepancy is evident from the 2D measurements which show much more spatially extended high-density regions than the modeling. The degree of the discrepancy can be quantified by averaging the density over the outer divertor volume (i.e., the region highlighted in panels a and b) and shows a density that is consistently $\sim 40\%$ less in the modeling than experiment across the three times analyzed (Table I).
Given this discrepancy, the persistence of the radiation deficit is not surprising as the radiated power is highly dependent on the electron density.

### IV. COMPARISON OF RADIATION CHARACTERISTICS WITH MATCHED DIVERTOR DENSITY

A second set of modeling has been performed focusing on matching the divertor density and temperature between modeling and experiment in order to test the role of parallel transport physics in contributing to the radiation deficit. This was accomplished by increasing the upstream electron density self-similarly while keeping the $T_e$ profile fixed, which has the effect of raising the divertor density, until the divertor-averaged electron density in the modeling agreed with the DTS measurement (Table I). This required upstream densities ~50% higher than measured. The resulting divertor $n_e$ and $T_e$ parallel profiles are shown in Figure 7. As can be seen, good agreement between the measured and modeled profiles is produced across the entire distance between the X-point and target surface, for both the density and the temperature. While the average divertor density is constrained to agree with measurements, the poloidal density gradient is not and so the degree of agreement in the gradient is noteworthy, as is the agreement in the electron temperature profile in the divertor, which is entirely unconstrained. Finally, as illustrated in Figure 8, while only a scalar quantity (the divertor-averaged $n_e$) is used to constrain the divertor parameters, good agreement is obtained in the full 2D distributions of $n_e$ and $T_e$.

These cases with the divertor density and temperature matched allow a more direct comparison of the radiated power for the purposes of evaluating the atomic physics involved. As shown in Figure 9, the total radiation in the outer divertor for these cases agrees very well with experiment for the highly radiating, high density cases, with modeling being within roughly 10% of the measured values. The degree of agreement is imperfect, in that the 2D distribution does not fully match experiment: as can be seen in Figure 10, the radiation pattern on the inner divertor leg is quite different between code and experiment (c.f. Figure 2(c)) and is likely attributable to the neglect of drifts which would tend to lower $T_e$ on the inner leg and hence strongly affect radiation. This confirms the focus here on the outer divertor, where measurements are available to ensure that

![Image](image_url)

**FIG. 6.** 2D profiles of (a) modeled and (b) measured electron density, and poloidal profiles along a near-separatrix flux tube for low density time slice. In panel (c), electron density versus poloidal connection length; $L_{pol} = 0$ indicates the outer target, and the X-point is located near $L_{pol} ~ 0.2$ m.

**FIG. 7.** Poloidal profiles of electron (a)–(c) temperature and (d)–(f) density for low (a) and (d), medium (b) and (e), and high (c), (f) density time slices for modeling cases with average divertor density matched to experiment.

<table>
<thead>
<tr>
<th>Time (ms)</th>
<th>$(n_e)_{av}^{\text{EXPT}}$ $(10^{19} \text{m}^{-3})$</th>
<th>$(n_e)_{av}^{\text{SOLPS Match upstream}} (10^{19} \text{m}^{-3})$</th>
<th>$(n_e)_{av}^{\text{SOLPS Match divertor}} (10^{19} \text{m}^{-3})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1600</td>
<td>3.9</td>
<td>2.7</td>
<td>3.5</td>
</tr>
<tr>
<td>2400</td>
<td>8.0</td>
<td>4.5</td>
<td>7.9</td>
</tr>
<tr>
<td>2800</td>
<td>11.3</td>
<td>6.9</td>
<td>11.2</td>
</tr>
</tbody>
</table>
the density and temperature profiles are well-reproduced in the modeling.

The result that helium modeling with a good match to the divertor density does not show an appreciable radiation shortfall confirms that 2D fluid models like SOLPS are in principle capable of quantitatively capturing the divertor radiation levels measured in experiment for the simpler case with helium as the main ion species. These results are also consistent with the efforts ongoing to improve the deuterium molecular physics set incorporated in the modeling, in that removing these uncertainties by running in helium also removed the large radiation discrepancy. However, these results also show that the larger challenge, at least in the helium experiments being analyzed, is achieving the experimental density and temperature throughout the divertor volume in the modeling, especially when only the upstream profiles are available from measurements.

V. IMPLICATIONS OF UPSTREAM MISMATCH

Although as described above the divertor density and temperature profiles from SOLPS agree very well with DTS measurements, the upstream profiles are no longer constrained to match measurement. This connection between the divertor and the main SOL is an outstanding issue and an open research area that will be necessary to understand in order to predict the divertor characteristics for given upstream parameters. Towards this end, it is instructive to inspect the degree of mismatch and explore possible sources of error, whether in the transport model itself, or through boundary conditions or other input to the model. Two major pieces of the overall SOLPS transport model are considered: the parallel electron heat transport model and parallel pressure or momentum balance. Each of these is central to the overall parallel collisional transport model that is employed in SOLPS.

As described above, SOLPS uses a fluid model for parallel electron heat transport, using classical collisional closures for the heat flux (also with kinetic corrections via flux limiters, although these are not important for the high collisionalities studied here). The electron component of the overall parallel heat transport is important since the classical conductivity is much higher for electrons than ions, by the square root of the electron/ion mass ratio. Figure 11 shows that the upstream electron temperature profile agrees very well with experimental measurement. Further, as described above, the poloidal temperature profile within the divertor region also agrees very well with measurements. This implies that, provided the power loss terms are accurately modeled (which is the case for these helium experiments, which show good agreement in the radiated power between code and experiment), the SOLPS model is sufficient to quantitatively describe the electron heat transport over the entire region from the main SOL near the midplane of the tokamak, all the way through the divertor to the PFC surface.

Of larger concern is the discrepancy in the measured electron density in the upstream SOL and that used in the modeling, with that latter being \(-50\%\) higher than experiment for all time slices considered for the cases with matched divertor density. This implies a potential issue with the parallel pressure balance, since the overly high electron...
density is effectively adding extra pressure to the upstream SOL. Pressure balance is a foundational concept in SOL physics, where the momentum and continuity equations can be combined to show that the total pressure should be constant along field lines, unless a strong momentum loss is present:

$$\frac{\partial}{\partial t}(p_e + p_i + n_i m_i V_i^2) = S_{\text{mom}} = m_i n_i V_i (\sigma v)_{\text{CX}} + S_{\perp}.$$ 

Momentum loss is expected due to collisions with neutrals and is expected to be strong at low electron temperature (<10 eV). Hence, one expects that within the divertor, where the neutral density is high and temperature low, pressure loss should be strong; otherwise, pressure can be expected to be constant along the magnetic field.

In the divertor region, SOLPS captures the pressure loss of the helium experiments well; this is shown directly in Figure 12 for the medium-density case, and the modest pressure loss of at most a factor of 2–3 is well-recovered for all time-slices modeled. This implies that the momentum loss due to friction of the plasma with the neutrals in the divertor is well-captured by SOLPS. Further, this has an important implication that, provided one can get the pressure modeled accurately near the X-point (i.e., at the entrance to the divertor), SOLPS provides a good quantitative model of the rest of the divertor to the PFC surface. It should be noted that the neutral density plays an important role in the pressure balance but that direct measurements are lacking at present. Discrepancy in the neutral pressure has also been identified as a contributor to radiation shortfalls in ASDEX Upgrade. Thus, while the agreement in the electron pressure here is promising, the role of neutral density should be explored more in the future to conclusively assess the sufficiency of this aspect of SOLPS.

The larger discrepancy is seen between the modeling and the values measured upstream near the crown of the plasma. As can be seen in Figure 12, the modeled upstream electron pressure is ~50% higher than is measured, as a result of the density discrepancy. This is similar to the “pressure hill” previously observed near the X-point in DIII-D experiments, where the electron pressure was measured to be higher than the upstream pressure. However, only the electron contribution to the pressure is measured here, whereas the pressure balance equation involves the total pressure including ion contributions both through the static ion pressure $p_i$ and the dynamic pressure $n_i m_i V_i$ due to parallel flow. This suggests that underestimating the ion contribution to the total pressure could be the source of the difficulty in simultaneously matching the divertor and the upstream density.

A missing ion pressure would take the form of either an ion temperature or flow speed being lower in the modeling than is measured in experiment. While, as stated above, ion temperature data are generally not sufficient in resolution to be used in the direct profile fitting procedures employed to match the upstream profile, some ion data are available to compare the modeling to. These measurements are made via charge exchange recombination spectroscopy, and since helium plasmas are under study here direct measurements of the main ion (i.e., helium) temperature are available (rather than relying on impurity ion carbon measurements as is typically done with deuterium plasmas). The ion temperature is indeed measured to be higher than is obtained from the modeling in the far SOL. Of note is that the measured $T_i$ is much higher than $T_e$ by a factor of nearly ten. Reaching this very high $T_i/T_e$ ratio is very challenging in SOLPS; as a check, even with simulations run with $\chi_i$ reduced to 0.01 m$^2$/s, $T_i$ was increased only slightly (and not much at all in the far SOL). This is because of strong energy exchange with the electrons; even with radial transport effectively turned off, the ions do not get substantially hotter than the electrons but instead transfer power to the electron channel. It should also be noted that kinetic effects may be quite important for ions in the main SOL, impacting especially the temperature anisotropy and the corresponding interpretation of diagnostics.

While direct SOL flow measurements were not a focus of this experiment, extensive literature exists on this topic from several tokamak experiments. These generally find very strong flows, approaching sonic ($M \sim 0.5$), in the main SOL. 2D fluid models such as SOLPS, on the other hand, predict essentially stagnant plasma flow everywhere outside...
of the divertor unless measures are taken to promote strong flows within the code. Reproducing the strong SOL flows measured is complex and requires additional assumptions on the nature of the cross-field transport (e.g., the simultaneous inclusion of an inward pinch velocity and poloidally asymmetric diffusion\(^\text{29}\)). This suggests that strong main SOL flows may also be contributing to the missing upstream pressure inferred from the modeling described here. While neither this nor the discussion of the ion temperature contributions above is conclusive (and is not meant to be so), these results do point to the need for more direct attention on ion temperature and flow in the main SOL, from both the experimental and modeling perspectives.

VI. DISCUSSION AND CONCLUSIONS

These overall results constitute a proof of principle that 2D fluid models such as SOLPS are indeed capable of quantitatively reproducing the radiated power level measured in the divertor. This is an important step, as it implies that the challenge to date in reproducing the radiated power is not universally present due to fundamentally missing physics in the models such as turbulence or strong kinetic effects. The analysis presented here relies heavily on direct electron density and temperature measurements throughout the outer divertor volume made with DTS, and only when these were modeled accurately could radiation shortfall be eliminated. These measurements have allowed the most direct test to date of the radiated power compared to experiment and are arguably required to study topics like the radiation shortfall quantitatively.

The absence of radiation shortfall in helium plasmas is consistent with the ongoing efforts to improve the atomic and molecular physics captured in modeling of deuterium plasmas; these results show that having complete atomic physics can lead to successfully reproducing the radiated power. However, further experiments and modeling of deuterium plasmas are required to show this conclusively, with direct measurements of the main radiating species (both deuterium and carbon emission in the case of the carbon-walled DIII-D). These efforts should include a focus on comparing the neutral density between code and experiment in order to better quantify and benchmark the neutral contributions to power and pressure balance. With carbon walls, carbon will be a major radiator at all divertor temperatures in deuterium plasmas, unlike the helium case, and so future efforts in this area should attempt to quantify both radiation channels\(^\text{30}\) and compare them to modeling as has been done here. Likewise, the same process of matching the divertor density and temperature profile will be required to conclusively compare radiation in deuterium plasmas. While this is left primarily to future research, we note that previous modeling of DIII-D experiments\(^\text{11}\) showed that the divertor density and temperature could be reasonably matched if the radiated power was artificially scaled to match experiment—consistent with the notion that there are missing contributions in the reaction set used in the modeling.

Finally, these results have also shown that 2D fluid modeling with SOLPS is able to quantitatively describe the plasma within the divertor but that the connection between the divertor entrance and the upstream SOL remains challenging. This has been worked around in the present modeling by increasing the upstream electron density to values higher than are measured, but future research should aim at better understanding the physics of this missing connection. Ion contributions to the total upstream SOL pressure have been identified as possible deficiencies in the current modeling, and further efforts towards measuring these in experiment and improving their treatment in modeling are warranted. Extending these ion studies to include the divertor region would also be of interest, since a mismatch in the ion parameters within the divertor could also in principle affect the overall comparison between measurement and modeling, for example, through the effect of ion parameters on sputtering yields. The very low carbon emission seen at high densities, however, suggests that these effects are not strong enough to substantially affect the radiation studies described here.

VII. SUMMARY

Experiments and modeling of dissipative divertor operation in helium plasmas at DIII-D have been performed to examine the possible role of molecular physics in the previously observed inability of models to reproduce the measured radiated power. By eliminating the uncertain and complicated molecular physics associated with deuterium, these experiments showed that the radiation can be fully accounted for in modeling. However, this required careful matching of the modeled divertor density to that measured; relying on upstream profile measurements alone (as is typically the case) resulted in lower density in the divertor and consequently lower radiated power than was measured. These results both demonstrate that fluid models are capable of quantitatively describing the divertor under simplified conditions and support the efforts that are ongoing to add the more complicated reactions needed to fully model deuterium divertor physics. Finally, this work has highlighted the need to improve the connection between the midplane and the divertor in the models in order to be able to predict divertor operation for given upstream conditions.

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