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*Published in:*
Nuclear Materials and Energy

*DOI:*
10.1016/j.nme.2019.01.019

Published: 01/05/2019

*Document Version*
Publisher's PDF, also known as Version of record

*Please cite the original version:*
UEDGE-predicted impact of molecules on low-field side target detachment in DIII–D

A. Holm⁎, A. Holm, M. Groth, T.D. Rognlien

Department of Applied Physics, Aalto University, Espoo, Finland
Lawrence Livermore National Laboratory, Livermore, California, USA

ARTICLE INFO

Keywords:
UEDGE
Molecules
Detachment
Fusion
Plasma
DIII-D

ABSTRACT

The impact of fluid molecules on detachment was studied using the edge fluid code UEDGE for a set of DIII–D L-mode plasmas with varying degree of low-field side (LFS) target detachment. A baseline atom-only, fluid-neutral model was compared to models including diffusive deuterium molecules with user-defined molecular temperatures and molecular temperatures solved via an energy equation, respectively. The UEDGE simulations including molecules with their temperature solved via the molecular energy equation displayed improved qualitative agreement with DIII–D measurements. However, at LFS separatrix electron densities below $1.3 \times 10^{19} \text{ m}^{-3}$ the LFS target peak electron temperature was over-estimated compared to the DIII–D measurements by a factor of 1.5–2. Kinetic effects, as the SOL collisionalities for LFS separatrix electron densities below $1.3 \times 10^{19} \text{ m}^{-3}$ are $\nu_{\text{coll}} \leq 15$, could contribute to this discrepancy. At LFS separatrix electron densities above $1.5 \times 10^{19} \text{ m}^{-3}$ UEDGE predicted LFS target peak ion current and electron densities a factor up to ∼ 4 lower than the DIII–D-measured values for all models. The consideration of molecules in UEDGE simulations induced a stable X-point MARFE, while an X-point MARFE was not achieved with the ion-atom model. The X-point MARFE forms due to a high-density front that connects the high-field side (HFS) and LFS divertor legs over the X-point, and is not observed for the atom-only UEDGE simulations. The high-density front forms due to molecular particle dynamics and cross-field drifts increasing the plasma density towards the X-point in the HFS leg.

1. Introduction

Future fusion power plants necessitate operation in an at least partially detached regime with low target temperatures (∼ 1 eV) and power fluxes (≦ 10 MW m⁻²) due to material limitations. The operational parameter space and divertor design required for operation under partial detachment are based on predictive numerical edge simulations. However, the plasma simulations are limited by the physics models included in the numerical codes. Thus, dedicated edge-code validation studies between codes, such as UEDGE, and experimental fusion devices, such as DIII–D, are required to verify the capability of the codes and allow confident extrapolation to future devices. UEDGE is a multi-fluid plasma code package, and the focus of this work.

Presently, discrepancies are observed between UEDGE predictions and experimental measurements in DIII–D [1,2]. Molecular deuterium processes, some of which are not yet included in UEDGE, are postulated to partially explain the differences [3]. Momentum and power losses due to molecular effects are postulated to increase the momentum losses and facilitate the onset of detachment [4–6]. Such effects include, but are not necessarily limited to, molecular assisted recombination, molecular radiation, and thermal equipartition of molecules with atoms and ions. The consideration of molecular deuterium also affects the particle balance and dynamics of the plasma, as each molecule is comprised of two deuterium nuclei which is dissociated volumetrically into atoms and ions. Thus, inclusion of a more detailed molecular deuterium model in UEDGE is expected to yield better agreement between code and experiment.

This work evaluates the UEDGE-predicted impact of including diffusive deuterium molecules in addition to deuterium atoms on low-confinement (L-mode) DIII-D plasmas. Two models for molecular temperature are considered: (M1) constant, user-specified value, and (M2) temperature solved via a molecular energy equation ($E_m$). The UEDGE predictions are subsequently compared to divertor Thomson scattering measurements in DIII–D, and the agreement between model and experiment is described.

The HFS target typically detaches at lower LFS midplane (LFS-mp) separatrix electron densities ($n_{\text{LFS-mp}}$) compared to the LFS target (LFS-t) due to drift effects when, as in this work, the ion VB drift is in the...
direction of the lower divertor [7]. Thus, this work focuses on LFS target detachment. This work defines plasma detachment as target electron temperatures $T^{LFS}_{e,\text{sat}} \leq 1$ eV accompanied by reduced peak ion current density to the LFS target ($J^{LFS}_{\text{ion}}$). Since the density at the LFS can be considered to define the scrape-off layer (SOL) boundary conditions, and is measured by the DIII-D diagnostics, this work considers $n^{LFS}_{\text{ion,mp}}$ as the independent parameter when considering the LFS plasma conditions.

2. Description of UEDGE model including atomic deuterium only (baseline)

A set of well-characterized, lower-single null DIII-D L-mode plasmas with the ion VB drift in the direction of the lower divertor [8,9] were modeled with UEDGE. These simulations include neoclassical drifts due to VB and $E \times B$ and their contributions to the particle radial and poloidal fluid velocities. Here, the direction of the ion VB drift is toward the lower divertor (forward toroidal magnetic field direction) resulting in higher-density, lower-temperature divertor plasma conditions in the HFS versus LFS divertor legs [10,11]. UEDGE implements a fluid treatment of the neutrals, which assumes the self- and plasma-collisionalities to be sufficiently high for validity of the fluid approximation. The simulations are run time-dependently with increasing time-step using a Krylov-Newton solver to achieve steady-state convergence, which was assured by evaluation at large-time-step with residuals within machine accuracy.

The UEDGE simulations were performed on an EFIT [12] magnetohydrodynamic equilibrium corresponding to DIII-D discharge 160299 at 2230 ms. The simulations consider deuterium plasmas with sputtered carbon impurities. At the core boundary, the ion and electron input powers are constant, $P_{\text{in,i}} = P_{\text{in,e}} = 0.45$ MW respectively, and the plasma density at the core boundary was taken as the independent parameter. The core boundary densities ($n_{\text{core}}$) were evaluated between the upper and lower density limits in increments of $10^{18}$ m$^{-3}$ until convergence could no longer be achieved. These intervals, for all models investigated, are presented in Table 1.

UEDGE solves the Braams transport equations [13,14] in the parallel and radial directions. The parallel plasma transport is taken to be classical, with imposed flux limits ($\chi_{i} = \chi_{e} = 0.2$, $\chi_{\gamma} = \chi_{\text{mol}} = 1$) approximating kinetic effects and preventing excessive VT-driven thermal transport. The imposed flux limits ($\chi$) approximately scale the corresponding classical diffusion coefficients by a factor $(1+|\chi^{-1}|)^{-1}$ [13]. Cross-field transport is assumed to be diffusion-driven and anomalous, with radially varying particle and heat diffusivities (in the ranges 0.75–6.6 m$^2$ s$^{-1}$ and 1.6–2 m$^2$ s$^{-1}$, respectively) vertically above the X-point according to Fig. 1. In the divertor, vertically below the X-point, the particle diffusivity is assumed spatially constant $D_{\chi} = 1$ m$^2$ s$^{-1}$. The corresponding heat diffusivities are $\chi_{i} = 0.75$ m$^2$ s$^{-1}$ and $\chi_{e} = 2$ m$^2$ s$^{-1}$ for ions and electrons, respectively. The global radial viscosity coefficient was taken to be $\gamma_{\text{vis}} = 2.6$ m$^2$ s$^{-1}$, the ratio of radial-to-parallel electric conductivity taken to be $10^{-8}$, and the convective coefficient used was 2.5.

UEDGE assumes strong charge-exchange coupling between the ions and atoms such that $T_{\text{e}} = T_{\text{i}}$, which allows the ion and atom energy equations to be solved as a single ion-atom fluid with a common temperature. UEDGE solves the continuity equation for all species present, solves a parallel momentum equation for the ions and electrons. Deterum atoms are described by charge-exchange diffusion across B-field lines and a full momentum equation along the magnetic field that includes inertia; this is referred to as the inertial neutral model. The potential equation is solved and the sheath potential contribution ($\text{ce}/T_{\text{e}}$) to the electron energy transmission factor ($\gamma_{\text{e}}$) is computed using the sheath conditions consistent with the parallel current at the plates [13]. The kinetic energy contributions to $\gamma_{\text{i}}$ and $\gamma_{\text{e}}$ are defined as 2.5 and 2 for the ions and electrons, respectively. Carbon impurities from physical sputtering at the target plates [15] and chemical sputtering at the target plates and radial grid boundaries from deuterium ions and atoms were considered. The chemical sputtering model used was the Haasz 1997 model [16] with low-energy corrections [13]. Strong Coulomb interaction is assumed between the deuterium and carbon ions and, thus, the carbon ion temperature is common to the deuterium ion temperature. The carbon model considers diffusive neutral carbon transport and treats ionic carbon transport using a force-balance model [13]. The carbon ions were fully absorbed at the target plates and grid boundaries, whereas the carbon atoms were fully recycled to mimic the recycling of hydrocarbons.

The baseline simulations include inertial deuterium atoms [13] only. The deuterium ions incident on the targets are recycled as deuterium atoms, and 1% of the one-sided, assumed Maxwellian, atom flux incident on the targets was removed. Dissociation is evaluated implicitly, since no molecular species are present in the simulation, by energy transfer from the electrons to the ion-atom fluid upon ionization. The Franck–Condon energy ($E_{\text{FC}}$), here taken as 5 eV, is gained by the ion-atom fluid, whereas the electrons lose half the dissociation energy ($E_{\text{diss}}$), here taken as $E_{\text{diss}} = 2E_{\text{FC}} = 10$ eV and, thus, does not include radiative dissociation losses.

3. Implementation of diffusive molecular deuterium models in UEDGE

Model 1 (M1) considers inertial deuterium atoms and rotationally relaxed, diffusive neutral deuterium molecules [17]. The deuterium atom and ion fluxes incident on the targets are recycled as molecules only: $0.5(I_{i} + I_{e}) = I_{\text{m}}$. As for the baseline, the one-sided, assumed Maxwellian, atom flux incident on the targets is removed at a 1% rate. Molecules are volumetrically dissociated into two atoms in the plasma through electron-impact [18], upon which the electrons transfer $E_{\text{diss}} = 2E_{\text{FC}} = 10$ eV to the ion-atom fluid. Thus, target recycling of deuterium ions and atoms is the sole molecular source and does not act as an atom or ion source. Rather, molecular dissociation and volumetric

Fig. 1. Radial profiles of the radial ion (red) and electron (black) thermal diffusivities and radial particle diffusion coefficient (green) vertically above the X-point. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
recombination are the considered atomic sources. The diffusive molecular flow is determined by the molecular elastic scattering rates $K_{m,j}$ of molecules with secondary species $j \in \{i, a, m\}$. Here, indices $i$, $a$, and $m$ refer to deuterium ions, atoms, and molecules, respectively, and the elastic scattering coefficients were assumed equal and constant at $T_m = 0.025$ eV, which models neutrals at approximately wall temperatures that do not interact thermally with the plasma. The defined, spatially constant temperature is an external boundary condition for power in the numerical domain as the energy carried by the molecules is transferred to the ion-atom fluid upon dissociation.

Model 2 (M2) is identical to M1, except that the molecular temperature is solved via a molecular energy equation. The molecular energy equation solved in UEDGE has the following form:

$$\frac{d}{dt} \left( \frac{3}{2} \rho_m T_m \right) + \frac{1}{V} \frac{\partial}{\partial x} \left( \rho_m u_x \frac{\partial T_m}{\partial x} \right) = \frac{V}{h_T} \frac{\partial}{\partial x} \left( \rho_m \frac{\partial y_m}{\partial x} \right) + \frac{1}{V} \frac{\partial}{\partial y} \left( \rho_m u_y \frac{\partial T_m}{\partial y} \right) = \rho_{eq,m,-}(T_m - T_c) + \rho_{eq,m,-}(T_c - T_m) + S_{\text{em}},$$

where $n_m$ and $T_m$ are the molecular density and temperature, respectively. Here, subindices $x$, $y$, and $\parallel$ refer to the poloidal, radial, and parallel directions, respectively, and subindex $m$ refers to the molecular species. The classical molecular velocity is represented by $v$, $u_x$, and $u_y$ which represents the total velocity with drift components included also, and $C$ is the convective coefficient. The heat conductivity and viscosity terms are given by $k_m = T_m\eta_{m\text{at},m\text{to},m\text{at}}$ and $\eta_m = T_m\eta_{m\text{at},m\text{to},m\text{at}}(w_{m,i} + w_{m,a} + w_{m,m})$ with applied flux limits, respectively. Here, $w_{m,i} = n_mK_{m,i}$ are the elastic scattering frequencies of molecules with secondary species $j \in \{i, a, m\}$, as above. The metric coefficients are $h_x = 1/\|Vx\|$ and $h_y = 1/\|Vy\|$, and $V = 2\pi R_b h_y$, $h_y$ is the volume element for toroidal geometry with major radius $R$.

The two first RHS terms of Eq. (1) describes the molecular sinks and sources due to thermal equipartition with species $j \in \{i, a, m\}$: $w_{eq,m,j} = \eta_{m\text{at},m\text{to},m\text{at}}$, where $V$ is the volume of the cell for which the equipartition is evaluated. The last term, $S_{\text{em}}$, describes the molecular energy loss through dissociation.

4. UEDGE-predicted impact of molecules on LFS target detachment

M1 displays similar qualitative behavior as the baseline: $I_{\text{LFS-max,peak}}^{\text{sat,peak}}$ decreases as a function of increasing $n_{\text{LFS-mp}}^{\text{sat,peak}}$. Both models have a local $I_{\text{LFS-max,peak}}^{\text{sat,peak}}$ maxima at $n_{\text{LFS-mp}}^{\text{sat,peak}} = 2.0 \times 10^{19} \text{ m}^{-3}$ (M1) and $n_{\text{LFS-mp}}^{\text{sat,peak}} = 1.4 \times 10^{19} \text{ m}^{-3}$ (baseline) (Fig. 2). The UEDGE-predicted $I_{\text{LFS-max,peak}}^{\text{sat,peak}}$ of M2 is qualitatively different from the baseline and M1. M2 converges over a wider $n_{\text{LFS-mp}}^{\text{sat,peak}}$-interval and displays a distinct $I_{\text{LFS-max,peak}}^{\text{sat,peak}}$-rollover at $n_{\text{LFS-mp}}^{\text{sat,peak}} = 2.0 \times 10^{19} \text{ m}^{-3}$ (Fig. 2). The M2-predicted $n_{\text{LFS-mp}}^{\text{sat,peak}}$ are also observed to saturate at high core densities due to the formation of an X-point MARFE [19], as discussed below. The vertical lines in Figs. 2–3 and 6 mark $T_{\text{LFS-max,peak}}^{\text{sat,peak}} \approx 1$ eV and represent detachment as $I_{\text{LFS-max,peak}}^{\text{sat,peak}}$ is decreasing at these points (Fig. 2).

The UEDGE-predicted detachment for M1 occurs at approximately $5 \times 10^{19} \text{ m}^{-3}$ lower $n_{\text{LFS-mp}}^{\text{sat,peak}}$ compared to the baseline and M2 (Fig. 2 and Table 1). The shift is due to the temperature and density dependency of the particle removal rates resulting in different LFS target particle removal rates as a function of $n_{\text{LFS-mp}}^{\text{sat,peak}}$ for the models evaluated. The UEDGE-predicted particle removal rate by albedo-like pumping at the targets is defined as the fraction $(1 - \alpha_m) = 0.01$, per Sections 2 and 3, of the one-sided Maxwellian flux incident on the target: $(1 - \alpha_m)n_jI_{\text{LFS-max,peak}}^{\text{sat,peak}}/2\pi m_j$, where $j$ refers to the pumped species, in this case atoms. Due to the recycling of deuterium atoms and ions incident at the targets as deuterium molecules for M1 and M2, the deuterium atom densities at the targets are low, resulting in lower particle removal rates at the targets. The lower particle removal rates increase the divertor neutral densities for M1 at similar $n_{\text{LFS-mp}}^{\text{sat,peak}}$ compared to the baseline, which explains the shift of the target profiles towards lower $n_{\text{LFS-mp}}^{\text{sat,peak}}$. Further work is necessary to determine why the same effect is not observed for M2, and to perform corresponding simulations using M1 and M2 with matching particle removal rates to isolate the effect of introducing molecules to the plasmas.

UEDGE predicts $\sim 50\%$ higher maximum carbon radiation for M1 and M2 compared to the baseline at the upper $n_{\text{LFS-mp}}^{\text{sat,peak}}$-limit (Fig. 3b). This is due to the formation of an X-point MARFE, as discussed below, which exhausts the power before it reaches the divertor leg, where hydrogen typically radiates. Thus, the X-point MARFE increases the carbon radiation in the numerical domain and decreases the hydrogen radiated power after detachment of M1 and M2 (Fig. 3a,b). The shift of $n_{\text{LFS-mp}}^{\text{sat,peak}}$ towards lower densities is also observed for the radiated power (Fig. 3a,b).

UEDGE predicts the formation of a stable X-point MARFE for M1 and M2, but not for the baseline, at $n_{\text{LFS-mp}}^{\text{sat,peak}}$ above the thresholds in Table 1 (Fig. 4). The MARFE persists as $n_{\text{LFS-mp}}^{\text{sat,peak}}$ is further increased to the upper $n_{\text{LFS-mp}}^{\text{sat,peak}}$-limit. In Figs. 4 and 5 the surfaces shown are taken at detachment, when $T_{\text{LFS-max,peak}}^{\text{sat,peak}} \approx 1$ eV for the respective model and are presented in Table 1. The corresponding densities for the drift cases are also marked by vertical lines of the color of the respective model in Figs. 2–3 and 6. The choice of $T_{\text{LFS-max,peak}}^{\text{sat,peak}} \approx 1$ eV as common parameter is motivated by the shift of the M1 profiles to lower $n_{\text{LFS-mp}}^{\text{sat,peak}}$ values, which makes $n_{\text{LFS-mp}}^{\text{sat,peak}}$ an unsuitable common parameter.

Inclusion of cross-field drifts in the models causes the electron densities to increase in the direction of the cross-field drifts [11], forming a high-density region over the X-point (Fig. 5). The inclusion of molecules in M1 and M2 increases the plasma density in the divertor region upstream towards the X-point at $T_{\text{LFS-max,peak}}^{\text{sat,peak}} \approx 1$ eV compared to the baseline when not considering drifts (Fig. 5a,b,c). This is due to the recycling of ions and atoms as molecules at the target plates, consideration of the molecular pressure gradients at the targets, and transport of molecules upstream towards the X-point where they dissociate into atoms. With increasing $n_{\text{LFS-mp}}^{\text{sat,peak}}$, the molecules are transported further upstream before they dissociate due to decreasing target electron temperatures (Fig. 6a), creating a volumetric atom source further upstream. The ionization of the atoms is a volumetric plasma source which locally increases the electron density. The ionization surfaces are similar to both the dissociation and electron density surfaces, indicative of molecular transport being responsible for a more even plasma density distribution, with increased plasma densities closer to the X-point compared to when molecules are not considered. The increased plasma density close to the X-point, due to molecular particle dynamics and cross-field drifts, results in a high-density front between the HFS and LFS divertor legs forming over the X-point for M1 and M2. Thus, the plasma and partially ionized carbon are restricted to the core region where carbon radiates power, creating an X-point MARFE. Increasing particle flow into the core region, due to the formation of a high-density front, can cause increased flow in the SOL, draining particles from the LFS-mp. This can explain the saturation of $n_{\text{LFS-mp}}^{\text{sat,peak}}$ when $n_{\text{core}}$ is increased sufficiently as observed for M2.

5. Comparison of UEDGE predictions against DIII–D measurements

Experimentally, the DIII–D discharges \(^1\) constituted L-mode density scans in the sheath-limited, high-recycling, and detached regimes to study the SOL and validate edge codes. The DIII–D lower divertor is covered by a comprehensive diagnostics system [20], of which the
The discharges were performed at fixed plasma conditions of the respective model. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The UEDGE-predicted \( t_{i,peak}^{LFS-t} \) of the baseline and M2 correspond well to the DIII-D measurements at \( n_{e,sep}^{LFS-mp} > 1.3 \times 10^{19} \text{ m}^{-3} \) (Fig. 2). Only the M2 \( n_{e,sep}^{LFS-mp} \)-interval extends to \( n_{e,sep}^{LFS-mp} < 1.3 \times 10^{19} \text{ m}^{-3} \) as also observed in DIII-D. At \( n_{e,sep}^{LFS-mp} < 1.3 \times 10^{19} \text{ m}^{-3} \) the M2 \( t_{i,peak}^{LFS-t} \)-predictions exceed the DIII-D-measured \( T_{e,DIII-D} \approx 30 \text{ eV} \) with a factor of 1.5–2. At such temperatures the molecular densities are insignificant in the divertor, except immediately in front of the targets where the incident ions and atoms are recycled as molecules, due to the strong volumetric molecular dissociation sink. Thus, the impact of including molecules at \( n_{e,sep}^{LFS-mp} < 1.3 \times 10^{19} \text{ m}^{-3} \) is considered insignificant, although the inclusion of a molecular energy boundary condition at the target plates in UEDGE alleviates the constraints on the numerical solver at lower \( n_{e,sep} \). The discrepancy at such \( n_{e,sep} \) might be due to kinetic effects as the SOL collisionalities (\( \nu_{\text{coll}} = 10^{-16} \text{ kg}^{-1} \text{s}^{-1} \)) are \( \nu_{\text{coll}} \leq 15 \), which could be alleviated by imposing stronger flux limits and adjusting the radial transport coefficients according to predictions by dedicated kinetic simulations.

The UEDGE-predicted LFS peak target electron densities (\( n_{e,sep}^{LFS,t} \)) at \( n_{e,sep}^{LFS-mp} > 1.5 \times 10^{19} \text{ m}^{-3} \) are a factor of \( \sim 4 \) lower than the DIII-D-measured values (Fig. 6b). The processes causing this discrepancy are not yet fully understood, but the same discrepancy has been replicated using the fluid-kinetic code EDGE2D-EIRENE [9]. The UEDGE-predicted \( n_{i,peak}^{LFS-t} \) for the baseline does not roll over, which is also observed

**Table 1**

<table>
<thead>
<tr>
<th>Densities [10^{19} \text{ m}^{-3}]</th>
<th>Baseline</th>
<th>M1</th>
<th>M2</th>
</tr>
</thead>
<tbody>
<tr>
<td>core-( n_{e,sep} )-interval</td>
<td>4.0–5.7</td>
<td>2.0–3.5</td>
<td>1.9–5.0</td>
</tr>
<tr>
<td>LFS-mp-( n_{e,sep} )-interval</td>
<td>1.7–2.3</td>
<td>1.1–1.9</td>
<td>0.7–2.3</td>
</tr>
<tr>
<td>( n_{e,sep}^{LFS-mp,\text{MARFE}} )</td>
<td>–</td>
<td>1.8</td>
<td>2.1</td>
</tr>
<tr>
<td>( \gamma_{i,peak}^{LFS-t} \approx 1 \text{ eV} )</td>
<td>(2.3)</td>
<td>(1.7)</td>
<td>(2.2)</td>
</tr>
</tbody>
</table>

The UEDGE-predicted LFS peak target electron densities (\( n_{e,sep}^{LFS,t} \)) at \( n_{e,sep}^{LFS-mp} > 1.5 \times 10^{19} \text{ m}^{-3} \) are a factor of \( \sim 4 \) lower than the DIII-D-measured values (Fig. 6b). The processes causing this discrepancy are not yet fully understood, but the same discrepancy has been replicated using the fluid-kinetic code EDGE2D-EIRENE [9]. The UEDGE-predicted \( n_{i,peak}^{LFS-t} \) for the baseline does not roll over, which is also observed

**Fig. 2.** UEDGE-predicted and DIII-D-measured LFS peak target current densities as a function of LFS electron separatrix density, \( n_{e,sep}^{LFS-mp} \). The cases shown in Figs. 4–5 are marked by the vertical lines for which \( T_{e,peak}^{LFS-t} \approx 1 \text{ eV} \) of the respective model. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Fig. 3.** Hydrogen (a) and carbon (b) radiation losses as a function of LFS electron separatrix density, \( n_{e,sep}^{LFS-mp} \). The cases shown in Figs. 4–5 are marked by the vertical lines for which \( T_{e,peak}^{LFS-t} \approx 1 \text{ eV} \) of the respective model. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
for DIII–D measurements within the range of the experimental data. Both M1 and M2 predict an $n_{\text{sep}}$-rollover, which qualitatively differs from the baseline predictions and DIII–D measurements. It should also be realized that the DIII–D measurements do not indicate the existence of an X-point MARFE, which is observed for M1 and M2.

6. Conclusions

UEDGE predicts the formation of a high-density front, connecting the HFS and LFS divertor legs over the X-point, due to molecular particle dynamics, resulting in a stable X-point MARFE when solving the molecular energy equation, $E_m$. The X-point MARFE is also observed at $n_{\text{sep}}^{\text{LFS-MARFE}} < 1.8 \times 10^{19} \text{ m}^{-3}$ when considering molecules of constant molecular temperature, but not for atom-only simulations. When molecules of constant $T_m = 0.025 \text{ eV}$ are included, UEDGE predicts $5 \times 10^{18} \text{ m}^{-3}$ lower $n_{\text{sep}}^{\text{LFS-MARFE}}$ required to achieve $T_{e,\text{peak}}^{\text{LFS-MARFE}} \approx 1 \text{ eV}$ compared to the atom-only model and when molecules with temperatures solved via $E_m$ are considered. This is postulated to be a result of varying particle removal rates for the different models due to the temperature and density dependency of the albedo-like pumping. The processes controlling the particle removal rates and its impact on the target conditions is not yet fully understood and subject to further investigation.

The inclusion of molecules with temperatures solved via $E_m$ improves the qualitative agreement between UEDGE predictions and DIII–D measurements of peak LFS target density, temperature, and electron density compared to atom-only and constant $T_m$ models. Quantitatively, all models evaluated under-estimate the peak LFS target electron densities and ion currents at $n_{\text{sep}}^{\text{LFS-MARFE}} < 1.7 \times 10^{19} \text{ m}^{-3}$ compared to DIII–D measurements by a factor up $\sim 4$. The processes causing the quantitative discrepancies are not yet fully understood, and subject to further investigation. UEDGE simulations using the molecular model solving $E_m$ converges at $n_{\text{sep}}^{\text{LFS-MARFE}} < 1.7 \times 10^{19} \text{ m}^{-3}$ whereas the constant $T_m$ and atom-only models do not. At such $n_{\text{sep}}^{\text{LFS-MARFE}}$-values, the molecular model solving $E_m$ over-estimates the peak LFS target electron temperatures by a factor of 1.5–2, which likely is due to kinetic effects as $w_{\text{kol}} \lesssim 15$. The $T_{e,\text{peak}}^{\text{LFS-MARFE}}$-agreement between UEDGE and DIII–D measurements at $n_{\text{sep}}^{\text{LFS-MARFE}} < 1.3 \times 10^{19} \text{ m}^{-3}$ could be improved by adjusting the radial transport coefficients and flux limits according to dedicated kinetic simulations. The model with molecular
temperatures solved via $E_m$ implemented in UEDGE will be verified against dedicated EDGE2D-EIRENE simulations to assess the agreement compared to a kinetic-neutral model.

Acknowledgments

This work was carried out under the Academy of Finland grant agreement No 285143. This work was supported in part by the U.S. DOE, Office of Science, Fusion Energy Sciences under Contracts DE-AC52-07NA27344 at LLNL and DE-FC02-04ER54698 at General Atomics. DIII–D data shown in this paper can be obtained in digital format by following the links at https://fusion.gat.com/global/D3D_DMP.

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