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A Validated Multi-Physics Modeling Approach to Predicting Erosion, Re-deposition and Gas Retention in Fusion Tokamak Divertors

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Plasma surface interactions between the edge of a magnetically confined plasma and the surrounding wall components lead to detrimental effects for both the wall materials and the plasma, including surface erosion, emission of impurities that radiate and dilute the plasma, loss of fuel through retention in the walls leading to materials property degradation, etc. Understanding and controlling these plasma-surface interactions (PSI) is therefore widely recognized as a critical need for realizing a fusion reactor. However, predicting PSI is challenging as these span diverse physical processes and many decades of time and length scales (ps–s and Å–m). Here, we present a simulation capability built to predict PSI: an experimentally validated suite of models that are integrated to capture the multi-physics nature of interactions between the edge plasma and the divertor surfaces in a fusion tokamak. This workflow includes SOLPS and/or experimental descriptions of the edge plasma in steady-state conditions; the effect of the electric and magnetic sheath at shallow magnetic angles modeled by the particle-in-cell code hPIC; the migration of impurities eroded from the divertor surface modeled by the impurity transport model in GITR; and the response of the divertor surface to these plasma conditions (gas recycling and implantation profiles, changes in surface morphology, effect of impurities in these processes, etc.), which is modeled by coupling the binary collision code F-TRIDYN and the cluster dynamics reaction-diffusion model, Xolotl.

We have validated the predictions of tungsten (W) net erosion, impurity transport and implanted gas concentrations from this workflow against dedicated experiments in the linear plasma device PISCES, which measured mass loss, tungsten spectroscopy and depth profiles of gas concentrations for long exposures of W substrates to various, low-energy mixed deuterium (D)- helium (He) plasmas: 100s of He plasma, 1000s of 10%He-90%D plasma and 3600s of D plasma, at 250eV bias voltage. For exposures to pure D plasmas, the model assumes a near-perfect W substrate containing 0.5% vacancies but no grain boundaries or other defects, and therefore underestimates the concentration of traps for the implanted D gas. This mechanism is less impactful in the presence of He clusters that act as strong traps, and therefore, the integrated model predictions of subsurface gas concentrations (Fig. 1, right) for exposures to mixed D-He plasmas are in good agreement with the experimental measurements (Fig. 1, left). As well, although not shown here, there is good agreement between the model and experiments for mass loss and W spectroscopy. The positive initial comparison against PISCES experiments (Fig. 1) instills confidence in the integrated model for predicting impurity migration, changes in surface morphology and gas recycling in the ITER divertor, under conditions expected for initial helium (He) and subsequent burning-plasma operations (BPO).

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For both ITER scenarios, SOLPS predicts standard strongly radiating, partially-detached plasmas in the divertor. Although our modeling predicts that much of the impact energy-angle distributions of light ions (D, T and He) are below the energy threshold for W sputtering, the high-energy tails extend well above this threshold. Under He operation, this sputtering leads to net erosion across the outboard divertor target, despite strong W re-deposition predicted by GITR, as depicted in Figure 2 (left). However, when accounting for changes in surface morphology caused by gas implantation, as predicted by Xolotl, the modeling indicates that the balance between erosion/re-deposition of W (predicted by GITR) and localized surface swelling driven by He implantation (predicted by Xolotl), results in surface recession far from the strike point (R-R_{sep}>0.15m) but at smaller magnitude than in GITR, and surface growth near the strike point (R-R_{sep}~0–0.15m), as shown in Fig. 2 (right).

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Under burning plasma conditions, Ne is the main radiative species and contributor to wall erosion. Over 90% of the eroded W locally re-deposits, which produces net deposition where the plasma temperature is low

 $(R-R_{sep}>0.15m)$ and net erosion where the plasma temperature is high $(R-R_{sep}>0.2m)$. The trend is the same after accounting for the contribution of implanted gases in Xolotl, but the surface growth increases by an order of magnitude due to He-D-T gas nucleation. The depth profiles of gases implanted in the W divertor are not strongly impacted by dilute impurities. However, heat fluxes significantly affect the sub-surface D and T concentration magnitudes, as well as the spatial profiles, since increases in substrate temperature (of up to 175K at the peak heat flux location) during steady-state operation lead to faster gas diffusion, resulting in higher outgassing, as well as permeation into the bulk.

We also evaluated the influence of pre-exposure of the W substrate to He plasma (from the He-operation) on the tungsten divertor response to burning plasma operation. In this case, the higher concentration of He and vacancy clusters near the surface locally increases the D and T concentration (relative to an initial crystalline W) and initially (<50s) reduces the permeation of hydrogenic species, consistent with findings in the PISCES experiments, while the long-term (>50s) concentration of gases in the bulk is unaffected by the pre-exposure.

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