Plasma-neutral interaction studies with OpenMC

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The transport of recycling atoms in magnetic confinement plays a key role in plasma-wall interaction, fueling, and diagnostics [1]. Performant and user-friendly tools are demanded to predict their behavior. This is becoming increasingly important as neutrals are relied upon to protect the wall from intense heat fluxes, and neutral diagnostics are relied upon for plasma control. These effects are most important in the edge, where the spatial profile of plasma properties is strongly varying, including both the high-confinement pedestal and the scrape-off layer. Here we examine neutral fueling in the pedestal from first principles, paying particular attention to the impact of neutral opacity. The potential for recycling-driven positive-feedback effects on a variety of pedestal shapes are also considered, as is the possibility of scrape-off layer broadening from charge-exchange interaction with ions. These studies showcase the usefulness of this new application of OpenMC, which brings with it advanced capabilities over the existing legacy tools for neutral particle simulation.

Recently, the OpenMC framework has been adapted for atomic physics [2], this work represents the first physics study using this new capability. OpenMC has been benchmarked against DEGAS2 [3] with respect to accuracy and performance with the inclusion of ionization and charge exchange reactions. Figure 1 shows the results of a full-mesh comparison using an NSTX-U equilibrium. The electron density, temperature, and ion temperature are chosen as flux functions mapped onto a magnetic equilibrium. The source of neutral gas at 3 eV is from two mesh elements near upper and lower strike points. This, among other benchmarks, demonstrates that the ionization and charge exchange reactions are faithfully captured in this version of OpenMC. This enables neutral simulations to be accelerated on GPUs, allowing many more particles for more reliable convergence of coupled solutions. With an eye toward higher fidelity representation of the wall, one of the most attractive features of OpenMC is the ability to make direct use of native digital engineering models for the wall via CAD. This higher-fidelity representation of the wall will enable more direct synthetic line radiation diagnostics and more accurate prediction of the wall's response to plasma deposition.

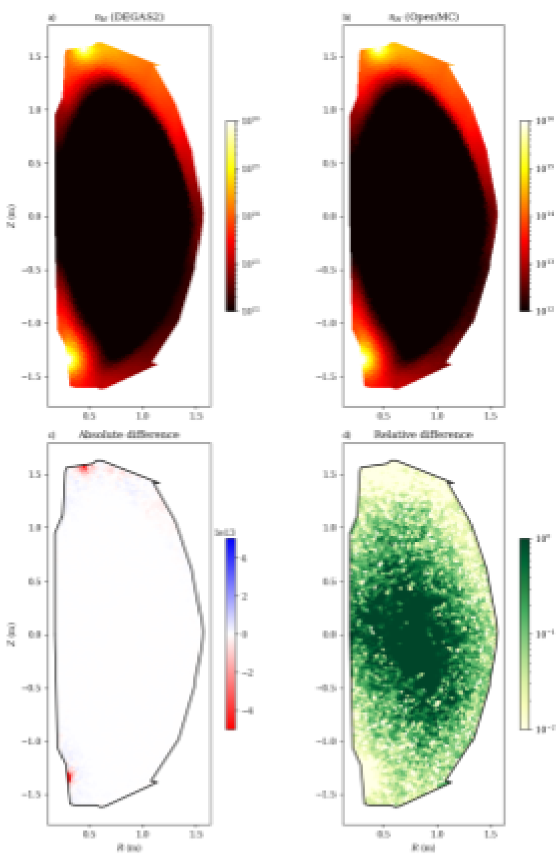

Figure 1. Comparison between calculated atomic density with DEGAS2 and OpenMC. a) and b) show the direct results for atomic density in DEGAS2 and OpenMC, respectively. c) shows the absolute difference between the two, with d) the relative difference. Reproduced from Ref. [2].

With this new tool, we perform a general study of the impact of neutrals on strong-gradient plasma regions. An ITER-like equilibrium is used as a base case for neutral simulations in a variety of plasma backgrounds, parametrized by 1D flux function profiles. Firstly, we scale the device size keeping all plasma properties consistent with normalized magnetic flux functions. The fueling efficiency, defined as the fraction of recycling neutrals that ionize inside the separatrix, is confirmed to decrease with larger device size [4]. It is further confirmed that the neutrals resulting from the charge exchange reaction are the dominant source of fueling, especially for larger devices.

As these neutrals ionize in the pedestal, several effects occur. Firstly, this acts as a particle source of electrons and ions in the pedestal. These particles typically have lower energy than the local plasma, therefore, there is not a proportional gain in plasma energy. Since the penetrating neutrals borrowed energy from ions closer to the edge, there is an additional sink of ion energy. How these effects interact with respect to the plasma gradients that drive pedestal instabilities is not obvious. We ran a series of simulations with several combinations of steep/shallow profiles of three quantities of interest: density and ion/electron temperature. The plasma sources in these quantities due to atomic interaction, together with their spatially-varying profiles, determines whether neutrals act to steepen or damp these gradients. If neutrals serve to steepen the gradient associated with the mode that limits pedestal structure, then one could expect a positive feedback mechanism. This would occur because increased plasma flux drives more recycling, leading to more ionization and to drive the gradients steeper still. It is found that, for this series of simulations, no pedestal structure is conducive to such a feedback loop with respect to pressure gradients. However, neutrals can drive η_i, the ratio between the ion temperature and density gradient scale lengths, associated with driving the ion temperature gradient mode.

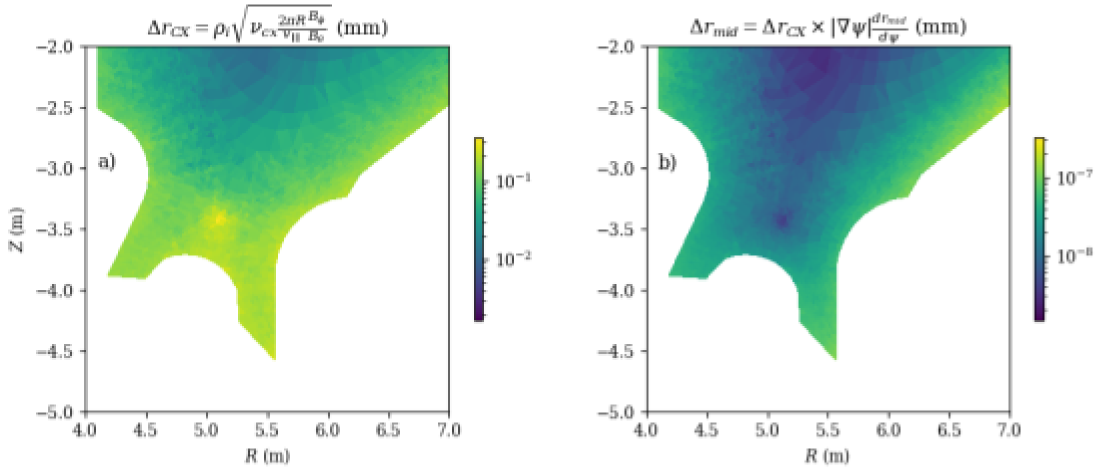

Figure 2. Illustration of the lack of SOL broadening from ion charge-exchange with recycling neutrals. a) shows the absolute local random-walk deflection in mm. b) shows the deflection by flux surface in terms of outer-midplane radius.

Finally, our attention is turned to the scrape-off layer, a region of even sharper plasma gradients. The possibility of scrape-off layer broadening due to ion interaction with recycling neutrals is investigated. The proposed mechanism is a random walk in steps of the ion gyroradius on time scales associated with the charge exchange reaction rate. In ITER, neutrals are expected to be most plentiful near the divertor. The ion interaction therewith is especially strong near the X-point, where the low magnetic pitch results in a relatively long dwell time for parallel-streaming ions. Figure 2(a) shows an estimate of the expected radial deflection from charge exchange interaction with neutrals. Unfortunately, it is found that flux compression between the X- and strike-points limits the impact of this mechanism, as shown in Figure 2(b). While the neutral density is sufficient to cause significant scrape-off layer broadening in an absolute and local sense, ions still follow magnetic field lines which converge toward the wall from the X-point, where this interaction is strongest. This is supported by full-F gyrokinetic edge simulations of ITER with XGC, which shows only a modest broadening of the ion wall deposition profile.

With these first physics results of neutral recycling using OpenMC, the community can look forward to more advanced applications that take advantage of digital representations of 3D wall structures, GPU acceleration, and a native C++ API that enables more straightforward coupling to other simulation software.

ACKNOWLEDGEMENTS

This work was supported by the U.S. Department of Energy under contract number DE-AC02-09CH11466 for the Princeton Plasma Physics Laboratory.

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