3D ASCOT simulations of ^{13}C transport in ASDEX Upgrade

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Introduction. In ITER, co-deposition of plasma fuel with carbon may lead to substantial retention of tritium. Therefore it is of utmost importance to learn how impurities such as carbon migrate in non-axisymmetric magnetic fields and accumulate on 3D wall structures. Most of the fluid-based global impurity transport codes typically assume axisymmetry for both the magnetic field and the tokamak wall structures. Local impurity transport codes, on the other hand, can operate in three dimensions with accurately accounting for the particle gyromotion, but they are limited to a small region of the wall surface.

ASCOT as a tool for impurity transport studies. ASCOT is a Monte Carlo particle-following code employing static magnetic and plasma backgrounds that can be extracted from experimental sources. It accurately accounts for all the neoclassical physics and can be operated with 3D wall structures and non-axisymmetric magnetic fields including toroidal ripple and RMP perturbations. ASCOT can trace guiding centers, Larmor orbits and, in the case of neutrals, ballistic orbits in an unrestricted computational domain. Coulomb collisions of the test particles with the background plasma are modelled using binomially distributed Monte Carlo operators derived from the Fokker-Planck equation [1]. These operators change the energy and the pitch of the test particle and, thus, are an a priori way of including such effects as friction, modelled by forces in the fluid approach. Anomalous transport in the radial direction is included using a diffusion operator. Until now, ASCOT has been mainly used for fast ion studies, most notably to estimate fast ion power loads on the plasma-facing components of ITER [2], but since it is not based on any assumption about particle energy or flux surface topology, we have now enhanced ASCOT with features that facilitate impurity studies in the open field lines of the scrape-off layer (SOL). The new features, described below, are i) charge-changing reactions for carbon, ii) plasma background flow, and iii) a model giving the impurities only a finite probability of remaining at the site of the original deposition. At the moment, the last feature consists of a model for impurity reflection (sticking coefficient $s \in [0,1]$).

i) Impurity transport studies require following not only charged particles but neutrals as well. To this end ASCOT is now refurbished with atomic physics: at each orbit-following time step, ASCOT calculates the probabilities, using the ADAS database, for effective ionization and recombination as the particle interacts with the background plasma. After neutralization the time stepping is taken along a ballistic path until either a re-ionization or an encounter with the wall.

ii) Earlier studies of ^{13}C transport in the ASDEX Upgrade (AUG) methane injection experiments were carried out using the DIVIMP code [3]. There it was found that the SOL background flow plays a key role: simulations using the self-consistent plasma backgrounds, created by the onion-skin model (OSM) solver, had the flow stagnation point at the top of the device and failed to reproduce the measured ^{13}C deposition distribution [3, 4]. It was only by imposing a background flow consistent with plasma flow measurements from various tokamaks [5], i.e., putting the stagnation point on the low-field side below the midplane, that made the simulated distribution resemble the measured one.

Since the collision operators of ASCOT assume a Maxwellian background plasma, they could be re-derived for a drifting Maxwellian distribution. Instead, we adopted the alternative route of carrying out a Lorentz transformation to the coordinate system moving with the bulk plasma each time the collisions are evaluated, and then transforming back to the laboratory frame.

iii) The first ASCOT results were obtained assuming that the first location where the impurity lands on a plasma-facing component will be its burial site, i.e., a sticking coefficient of unity was assumed. This is clearly an unrealistic assumption: not only do the impurities have a finite probability of getting reflected but, especially at the protruding elements, the probability of getting eroded due to the plasma exposure can be significant.

The most recent ASCOT enhancement introduces a probabilistic model for test particle reflection from wall surfaces. In the results reported in this contribution, a simple reflection is assumed, i.e., an elastic collision with the wall with a constant sticking coefficient. This model will be replaced by a more sophisticated model using data from the TRIM code to calculate the sticking coefficient as well as the energy and the direction of velocity of the reflected particle.

ASCOT simulations of the methane injection experiments. During the last experimental day of the 2007 campaign on AUG, isotopically labelled methane, $^{13}CH_4$, was injected into a series of L-mode plasmas, and a set of wall tiles was subsequently removed for surface analyses with secondary ion mass spectrometry. Less than 10% of the injected carbon could be accounted for by assuming toroidally symmetric deposition [4]. The experiments are described in detail in Refs. [3] and [4].

Figure 1 shows the ^{13}C distribution on the AUG wall, as calculated by ASCOT-PWI, for the methane injection experiment. The simulations were carried out for the discharge #22575 at 2.8 s, with $B_t = -2.5$ T and $I_p = 800$ kA. A total of 300 000 test particles were launched in sector

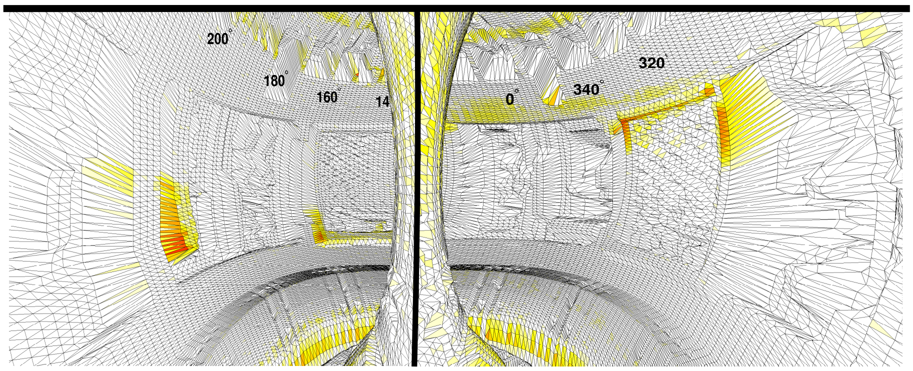
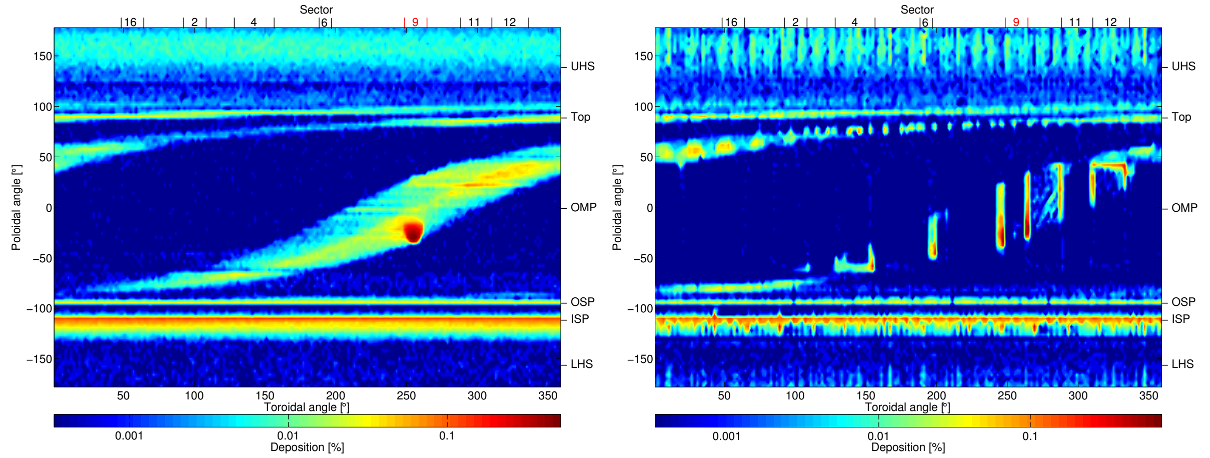


Figure 1: A panoramic view of ^{13}C deposition on the AUG first wall in the global methane injection experiments of 2007 as calculated by ASCOT-PWI when both the toroidal ripple and the true-to-life 3D wall are included. The colors indicate deposition relative to the total number of deposited particles on a logarithmic scale.

9 as a cylindrical cloud of $^{13}C^{1+}$ ions with roughly the size of the injection port and a radial thickness of 5 cm starting at the separatrix and extending outward in major radius. Thus, the full methane break-up chain was not modelled. The coefficient of anomalous radial diffusion was set to a constant value of $D = 0.25$ m^2/s. The background plasma in the main SOL was constructed using the OSM solver of DIVIMP, while the halo plasma was approximated by exponentially decaying profiles. According to the simulation results shown in Fig. 1, the assumption of a toroidal symmetry is clearly not justified in the main chamber. In particular, protruding wall structures, such as port and antenna limiters, are found to cause localized deposition patterns.

Figure 2 gives a more quantitative estimate for the significance of the 3D effects. The simulation results in Fig. 2(a) show the deposition distribution when both the magnetic field and the first wall structure are assumed axisymmetric, while in Fig. 2(b) the 3D AUG wall, also used in the results of Fig. 1, was applied, and the magnetic field had its rippled nature due to the finite number (16) of the toroidal field coils. In the purely axisymmetric situation, a large amount of the carbon is deposited in the neighbourhood of the injection location in sector 9, with weak but long wings extending in both directions along the field lines. Strongest deposition is observed at the inner divertor. Regions of weaker deposition are the outer divertor, the heat shield and the top of the vessel. When the 3D nature of the wall (and the field) is taken into account, the injection location can no longer be distinguished from the ^{13}C distribution but, rather, the shapes of the various limiter structures are visible in the deposition pattern. In both cases, however, the divertor deposition is rather accurately toroidally symmetric.

Repeating the simulations with a sticking coefficient of 0.7 mainly made the deposition more



(a) (b)

Figure 2: The 'unfolded' AUG first wall with ^{13}C deposition as calculated by ASCOT-PWI. (a) Assuming an axisymmetric wall, and (b) with the full 3D features of the wall. In both cases, the experimentally motivated flow of Mach = 0.5 towards the divertor plates, with a stagnation point halfway between the outer midplane and the X-point, has been used.

diffuse, most clearly at around the protruding elements. The result is intuitive – a reflected particle has a high probability of getting deposited not too far from its site of reflection.

Conclusions. The 3D structures of the first wall cannot be neglected when calculating the deposition of impurities in a tokamak environment. In particular, analyzing carbon deposition on tiles at just one toroidal location and assuming the same deposition on all tiles at that poloidal location can give orders of magnitude too high or low estimates for the total deposition, depending on the location. Including a constant sticking coefficient of $s = 0.7$ in the simulation model does not change this result quantitatively. Forthcoming studies will investigate the effect of erosion of deposited particles on the deposition pattern.

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References

[1] A. H. Boozer and G. Kuo-Petravic, Phys. Fluids **24**, 851 (1981)

[2] T. Kurki-Suonio et al., Nucl. Fusion **49**, 095001 (2009)

[3] T. Makkonen et al., J. Nucl. Mater., DOI: 10.1016/j.jnucmat.2010.08.023

[4] A. Hakola et al., Plasma Phys. Control. Fusion **52**, 065006 (2010)

[5] N. Asakura et al., J. Nucl. Mater. **363–365**, 41 (2007)