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SIMULATION OF NEUTRAL ATOMS AND MOLECULES IN AN INTERNATIONAL THERMONUCLEAR EXPERIMENTAL REACTOR HIGH-PRESSURE (1-Torr) ULTRAHIGH RECYCLING DIVERTOR

DIVERTOR SYSTEMS

KEYWORDS: *recycling, Monte Carlo modeling, ITER*

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The Monte Carlo code DEGAS was used to investigate the neutral atom and molecular interactions for a high-pressure (~1-Torr) gaseous divertor in the International Thermonuclear Experimental Reactor (ITER). Energy is removed from the plasma by radiation while the plasma pressure is balanced predominantly by a high neutral pressure at the end of the divertor. Plasma parameters were taken from the two-dimensional fluid code PLANET. Neutral sources from both ions recycling off the walls and recombination were included. The neutral density peak calculated with DEGAS of 3.43 ± 0.01 × 10^{22} m^{-3} occurred 4.5 cm from the divertor channel end. The ion and neutral atom energy fluxes were calculated to determine the heat load onto the divertor walls. A code was written to calculate the radiation distribution onto the side walls, not including any radiative absorption or reemission. The total energy flux peak (including ions, neutrals, and radiation) was 4.28 ± 0.30 MW/m^2. This falls below the design criteria of 5 MW/m^2. These results may help determine the wall material, heat removal, and the vacuum pumping requirements for the ITER divertor design and show the importance of a full treatment of neutral atoms and molecules in these regimes.

INTRODUCTION

A key concern in deuterium-tritium (D-T) fusion in the International Thermonuclear Experimental Reactor[1] (ITER) is heat exhaust. The power from charged particles is 300 MW out of 1500 MW total from D-T fusion. Exhausting heat without introducing impurities into the core plasma is a significant problem that the divertor must solve.[2] It must also be able to withstand the intense flux to the side walls due to the cross-field diffusion of charged particles, charge-exchange fast neutral atoms, and photons from a variety of radiative processes by staying below the proposed maximum energy flux of 5 MW/m^2. Sputtering of the wall must be minimized to ensure the lifetime of the wall and the purity of the core plasma.

Several mechanisms exist for removing energy from the divertor. In a high-recycling divertor, upward of 100 ion collisions occur with the plate for each ion that enters into the divertor channel. This occurs from ions hitting the plate and reflecting as molecules. The molecules transport through the divertor until they either ionize or dissociate and then eventually become an ion again. This process repeats until the molecule is lost to the pumps. The high-recycling regime typically takes place in a thin layer within 1 cm of the wall.[3]

Lengthening the divertor channel and injecting a pocket of cold neutral gas (puffing) perpendicular to the plasma flow in the divertor end is a method used to increase the amount of charge exchange and thereby decrease the temperature and flux of the fast ions. The scrape-off layer (SOL) plasma can be extinguished before reaching the plate with a high enough neutral density.[4] This detachment of the plasma may transfer more energy and momentum to the side walls instead of to the plate.[3] Simulations of the edge plasma in this type of divertor lead to two possible regimes: (a) an ultrahigh recycling regime characterized by high neutral pressures on the order of 1 Torr where recombination dominates,[5] and (b) a gas-target regime at only 10 mTorr where momentum is transferred to the side walls.[6] The goal of this

study is to investigate the ability of the ultrahigh recycling regime design to properly meet these criteria. Although the fluids codes contain neutral species, their accuracy in simulating neutrals under these conditions is poor. The fluid codes do not consider the changing mean free paths for interactions over the entire plasma volume or contain molecules and their reactions with the plasma. They also do not treat the neutral-wall interactions or sources properly. By coupling the fluid plasma solution to a full Monte Carlo treatment of neutrals, the veracity of the ultrahigh recycling regime solution can be discovered. A companion paper[7] investigates the veracity of the gas target regime solution.

MODELING

The two-dimensional PLANET fluid code[8] was used to model the plasma. The results of that modeling have been previously published[5] and are briefly described later. PLANET generates a self-consistent plasma state based on the following conservation equations:

1. electron energy
2. ion and neutral energies
3. electron mass
4. ion and neutral parallel momentum
5. neutral mass
6. neutral momentum normal to the field within the flux surfaces
7. neutral momentum in the radial direction.

The boundary conditions used are as follows. At the plate the heat transport is purely convective, and the pressure drops to zero over a boundary volume. Once a plasma is established in the iterative solution to the coupled differential equations, the particle flux on the main plasma boundary is set to zero. On the private flux side wall of the outer divertor leg, the plasma flux is set to zero. There is an input to the entire divertor of 330 MW, of which 220 MW entered the outer divertor SOL. Figure 1 shows the location of these regions and the geometry of the simulation. The neutrals modeled are atoms; molecules are left out. Also, the atom temperature is taken to be the same as the ion temperature. No gas puffing was used.

The mesh sizes below the separatrix were too large for proper convergence of the solution, so the data on the private flux region side of the separatrix are of limited validity.[9] However, the main purpose of this study is to calculate the particle and energy fluxes to the SOL side wall. Since the mean free path for neutrals is small, the plasma values in the private flux region do not influence the SOL fluxes. The plasma density and electron and ion

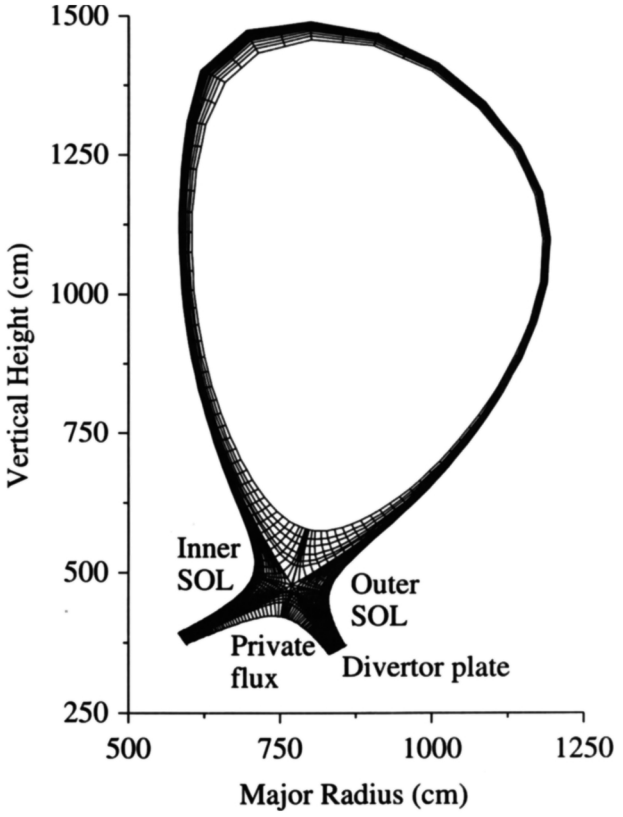

Fig. 1. Geometry mesh used in the PLANET code.

temperatures from this PLANET solution[5] were used as input for the DEGAS code.[2]

DEGAS is a three-dimensional Monte Carlo multispecies neutral transport code that contains extensive atomic physics, including charge exchange, electron and ion impact ionizations, and molecular dissociations. Energy- and angle-resolved wall reflection coefficients include effects of surface roughness and are taken from the fractal TRIM (transport in matter) code.[10,11] The source rate of neutral atoms is adjustable. It can originate from the flux of ions to the divertor side walls and plate, from gas puffing out of the side walls and plate, or from recombination within the plasma. The DEGAS geometry, taken exactly from part of the PLANET geometry, is shown in Fig. 2. The separatrix, x point, private flux, and SOL regions are labeled.

Figures 3, 4, and 5 show contours of the ion and electron temperatures and their density (which are equivalent). The upstream density at the midplane is 2×10^{19} m^{-3}. Neutral particles are sourced two ways: ion-electron recombination and neutral recycling from the ion flux to the walls. Separate runs were made for each case, and the results are summed, although only 0.1% of the atoms and 0.5% of the molecules produced were from recycling ions. In the recombination case, neutrals are sourced in the plasma according to the reaction rates in

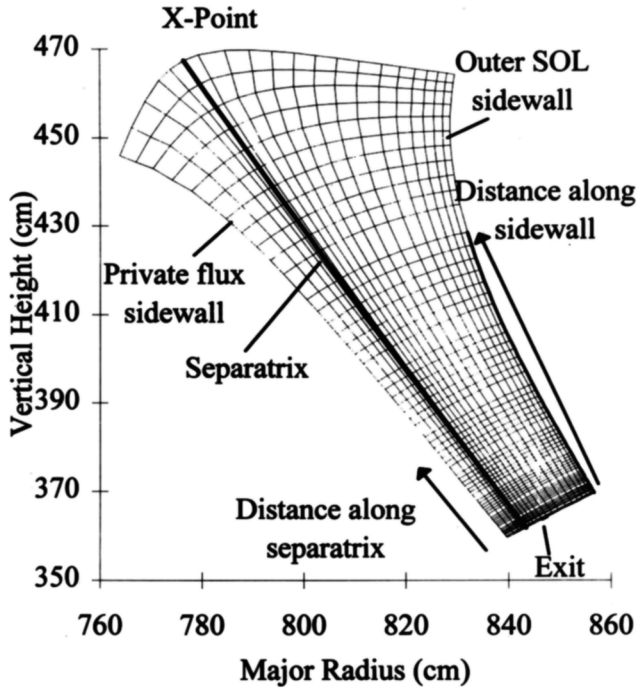

Fig. 2. Geometry mesh used in the DEGAS code.

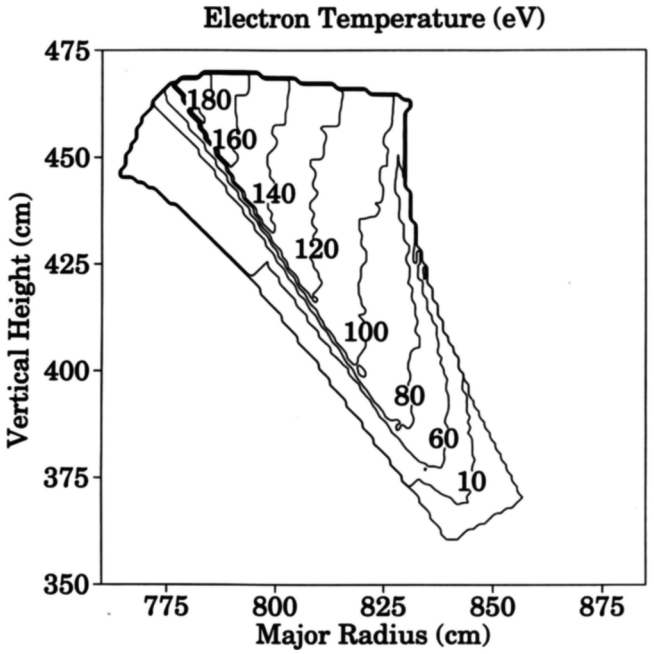

Fig. 4. Contours of the electron temperature.

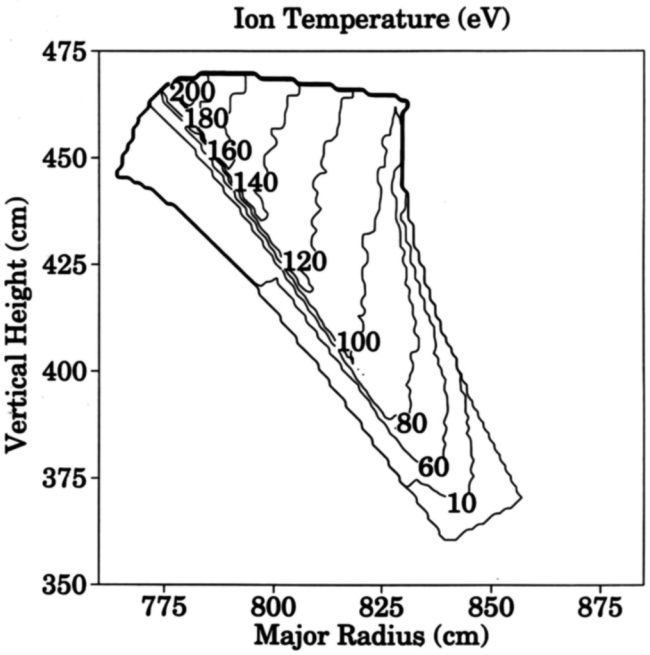

Fig. 3. Contours of the ion temperature.

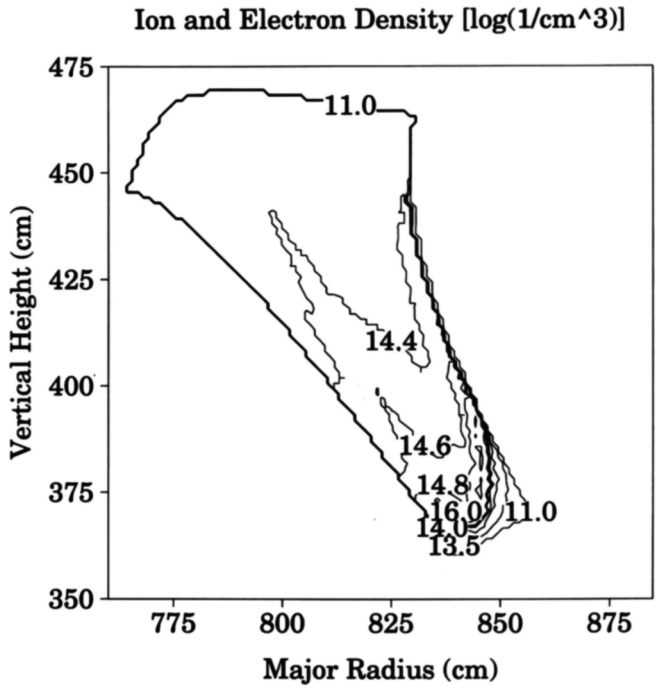

Fig. 5. Contours of the plasma density (ion and electron).

the code involving the ion and electron temperatures and densities:

$$\text{volume source rate} = \langle \sigma v \rangle (T_e) n_e^2 \ , \qquad (1)$$

where $\langle \sigma v \rangle$ is the reaction rate as a function of electron temperature and n_e is the electron density. In the recycling case, neutrals are sourced as a function of the ion flux, which is shown in Fig. 6. Each ion that strikes a wall is reflected off the wall as a neutral molecule. No neutrals are born in the plasma. The ion flux to the side wall (and perpendicular to the field lines) is

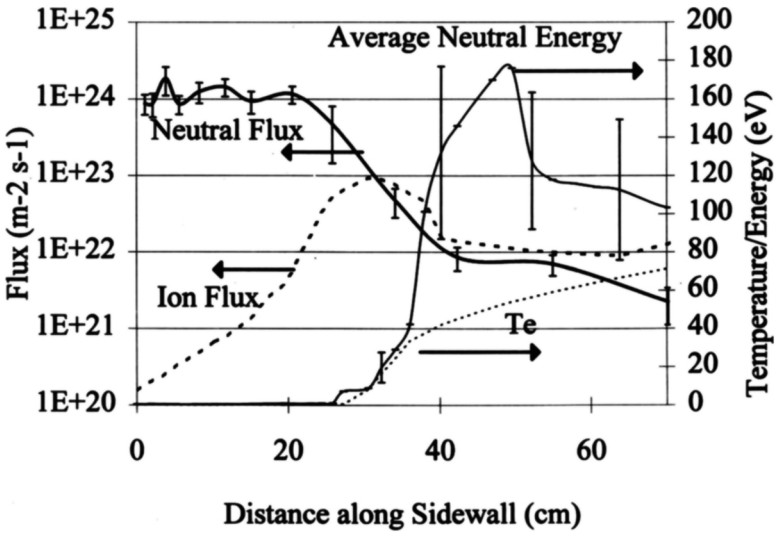

Fig. 6. The neutral atom flux and energy, the ion flux, and the electron temperature as a function of the distance from the divertor channel end along the side wall.

$$\Gamma_{ion} = \frac{1}{6} n_i \left(\frac{T_i}{M} \right)^{1/2} , \qquad (2)$$

where the subscript i denotes ions and M is the ion mass. The quotient of 6 is a crude model of the flux coming out of one side of a cube facing the wall.[9]

This simulation has a beryllium wall with an exit at the divertor channel end to model a pump duct. The upper divertor boundary is "mirrored"; that is, the same amount of neutral particles that cross it in one direction return with the same distribution. This has little effect since the hot plasma in that region prevents neutrals from approaching the boundary. The two-dimensional input is taken to be cylindrically symmetric. This has a negligible difference compared with toroidal symmetry for this size of device.

A code is developed to calculate the radiation distribution onto the divertor walls. It is to be used as a postprocessor with DEGAS. The values for the h-alpha production, the geometry, and the input power to the divertor are used as input. The h-alpha production rates are calculated in DEGAS, the geometry used is the same as in DEGAS, and the input power is calculated in the fluid code (in this case, PLANET). The result is a distribution of power density from the radiation onto the divertor side walls.

The h-alpha rate is calculated in DEGAS for comparison with actual experiments. Such h-alpha radiation is detectable with photodiodes, which are a common diagnostic for tokamaks. Lyman-alpha radiation carries the vast majority of the heat and power in a divertor, but it is not detected. DEGAS calculates the detectable h-alpha radiation for comparison to experiment. The rate of Lyman-alpha radiation production, however, is proportional to the h-alpha production. The power emitted from radiation is calculated by subtracting the ion and neutral power to the walls from the total power entering into the divertor. These are the three main processes for power to dissipate in the divertor. This value for radiation must equal the integral of the radiation to the walls over the surface area of the walls; thus, there is a mechanism for normalizing the h-alpha distribution to the effective Lyman-alpha distribution.

RESULTS

The neutral flux and neutral energy calculated for the outer divertor side wall are shown in Fig. 6 as a function of the distance from the divertor channel end. The input electron temperature and the ion flux are shown for comparison. The neutral density calculation from DEGAS and PLANET along the separatrix is illustrated in Fig. 7 together with the ion density. The distance along the separatrix begins at the end of the divertor channel and continues as illustrated in Fig. 2.

The neutral gas in the divertor channel end meets with the ions flowing in from the plasma. This creates a high recombination-ionization region, called the flame front. This is outlined by the 10-eV contour in Fig. 3. The neutral density drops where the ion density peaks, at ~5 cm from the plate. Figure 8 shows the ionization and recombination rates averaged along the separatrix to highlight the peaks for both PLANET and DEGAS calculations. No associated error for the PLANET results is supplied; hence, the recombination rate in DEGAS has no associated error since it is calculated as a function of input quantities from PLANET.

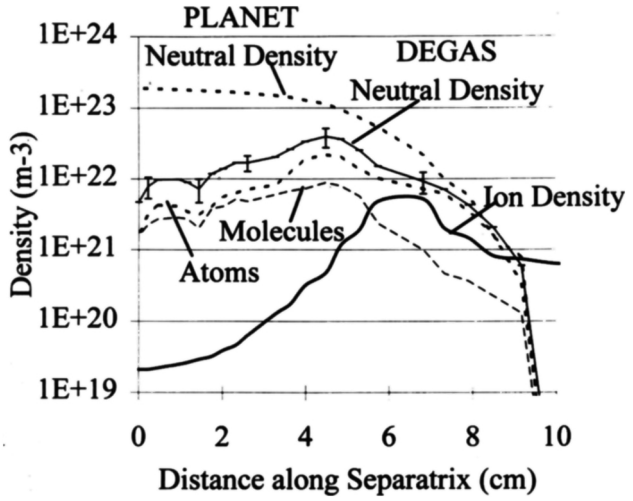

Fig. 7. The density of PLANET atoms, DEGAS atoms and molecules, and the ions as a function of distance from the divertor channel end along the separatrix.

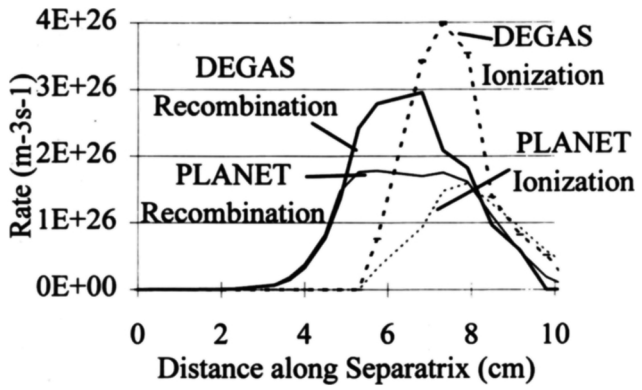

Fig. 8. The ionization and recombination rates for DEGAS and PLANET runs.

The ion energy flux is calculated as follows:

$$P''_{ion} = E \cdot \Gamma_i \tag{3}$$

and

$$P''_{ion} = \left(3T_e + \frac{1}{2}T_i\right)\frac{n_i}{6}\left(\frac{T_i}{M}\right)^{1/2} , \tag{4}$$

where E is the ion energy, n_i is the ion density, and M is the ion mass. The $3T_e$ term is due to a sheath, while the $\frac{1}{2}T_i$ term is due to a presheath. The power densities and their sum are shown in Fig. 9. The radiative power density peak of 4.21 ± 0.29 MW/m^2 is 10.5 cm from the end of the divertor channel, and the total power density peak of 4.28 ± 0.30 MW/m^2 is 11.9 cm from the end.

The energy and angular distributions of the neutrals colliding with the SOL side wall between 12 and 36 cm

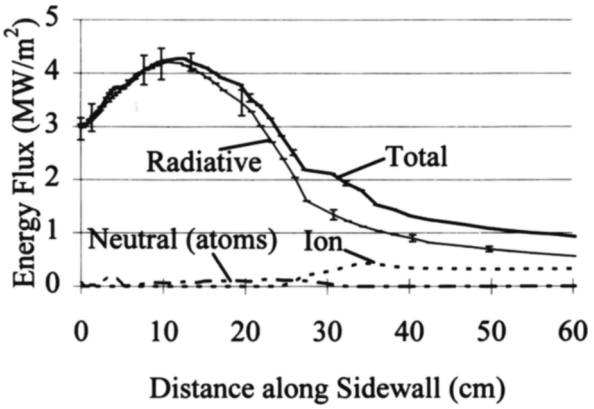

Fig. 9. The energy flux of the photons, atoms, and ions as a function of the distance from the divertor channel end along the side wall.

are graphed in Figs. 10 and 11. Note that the vast majority (89%) of the neutrals are <1.3 eV, and the plurality comes in at an angle between 36 and 54 deg. The neutral flux drops greatly when the neutral energy increases, as Fig. 6 illustrates. These low-energy neutrals are not a significant source of erosion, indicating that the vast majority comes from the ion flux. This is investigated in detail in Ref. 12.

DISCUSSION

The fluid solution for the neutral density is ~20 times that of the DEGAS solution in the region near the divertor channel end, as shown in Fig. 7. Past that region they

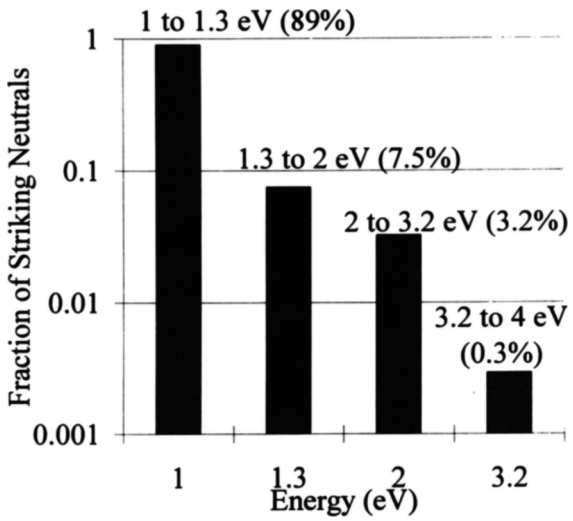

Fig. 10. Energy distribution of neutrals hitting the SOL side wall.

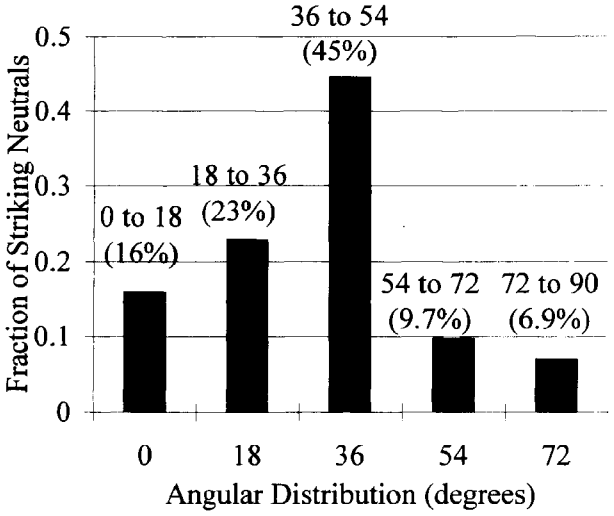

Fig. 11. Angular distribution of neutrals hitting the SOL side wall.

match closely, but the magnitudes are much less. However, PLANET equates the atom density and temperature to that of the ions and assumes equal parallel velocities for the ions and atoms. The consequence of this is that the plasma cannot flow through the neutral gas; only the neutral gas can diffuse through the plasma. These technicalities prevent a steady-state convergence.[5] The amount of neutral gas was taken to be constant with no pumping in the fluid simulation. This oversimplifies the divertor concept since it is only through the divertor that particles are pumped out. Neutral particles peak along the endplate in the PLANET simulation, whereas the DEGAS simulation includes an exit at the divertor channel end where neutrals leave the device. This density peak occurs 2 cm downstream from the recombination peak along the separatrix.

The exit makes up 6% of the simulation wall at the divertor channel end. The exiting flux of neutrals is 4.72×10^{20} atom/cm^2 and 7.38×10^{18} molecule/cm^2. This is 56% of the total neutrals sourced in the simulation. This exiting of the particles leads to a drop in the density near the divertor channel end. It is in this region that the discrepancy of the neutral density with the PLANET solution, which confines all the particles, is the greatest, as shown in Fig. 7.

The ionization rate in the DEGAS simulation has a maximum that is more than twice that of the PLANET simulation (see Fig. 8). The higher ionization creates a larger sink for the neutrals, thus lowering the neutral density. This occurs 7 cm from the divertor channel end, which is the same place the DEGAS neutral density begins to drop relative to the PLANET density (see Fig. 7). Some of the differences in ionization and recombination rates can be attributed to the different atomic physics that each code uses. An upgraded package is incorporated into DEGAS.

PLANET ignores molecules, while DEGAS includes a full treatment of the molecules with electron impact ionization, molecular dissociation, and dissociate ionization. Atoms penetrate several centimetres through the ionization front into the plasma, whereas molecules do not.

The Monte Carlo method has distinct advantages in calculating the neutral transport throughout a plasma. The DEGAS neutral solution is dependent on the plasma it interacts with as opposed to chosen boundary conditions that the neutral fluid solution is dependent on. PLANET has likely overestimated the neutral density, considering the assumptions made (ion and neutral flows and temperatures being equal) and simplifications taken of relevant processes (no pumping and lack of molecules).

The results for the energy fluxes to the side walls are within acceptable limits. The peak power density to the side wall surface is 4.28 ± 0.30 MW/m^2 at 11.9 cm, which falls below the design criteria of 5 MW/m^2. Radiation is the major carrier of the power, which is why the distribution is not decisively peaked at any one point but rather gradually increases to the side wall where the ionization-recombination flame front is. It appears that this high-recycling divertor solution will adequately spread the power from the plasma to the side walls of the divertor through radiation and conserve momentum through the existence of a high neutral pressure, but it may be unacceptable because of erosion concerns from the high ion flux.

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