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Self-Consistent Coupling of DSMC Method and SOLPS Code for Modeling Tokamak Particle Exhaust

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Abstract. In this work, the investigation of the neutral gas flow in the JET sub-divertor area is presented, with respect to the interaction between the plasma side and the pumping side in the sub-divertor region. The edge plasma side is simulated with the SOLPS code, while the sub-divertor area is modeled by means of the Direct Simulation Monte Carlo (DSMC) method, which in the last few years has been proved able to well describe rarefied, collisional flows in tokamak sub-divertor structures. Four different plasma scenarios have been selected and for each of them a manual, iterative procedure between SOLPS and DSMC has been established, using the neutral flux as the key communication term between the two subsystems. The goal is to understand and quantify in a self-consistent manner the mutual influence between the two codes, namely, how the particle exhaust pumping system controls the upstream plasma conditions. Parametric studies of the flow conditions in the sub-divertor side, including additional flow outlets and variations of the cryopump capture coefficient have been performed as well, in order to understand their overall impact on the flow field. The DSMC analyses resulted in the calculation of both the macroscopic quantities, i.e. temperature, number density and pressure, and the recirculation fluxes towards the plasma chamber. A slight deviation with the recirculation rates assumed in SOLPS has been found.

1. Introduction

In this paper, the neutral deuterium gas flow behavior through the JET divertor is investigated by coupling two well-established numerical approaches, namely the SOLPS code package and the direct Simulation Monte Carlo (DSMC) Method. In the last few years, lots of effort have been put trying to properly model the neutral gases flows in the divertor and sub-divertor areas in tokamak fusion reactors, for the neutral dynamics heavily influences the exhaust pumping process and the overall pumping efficiency. Nevertheless, from both the physical and the engineering point of view, the description of gas dynamics in the divertor and in the vacuum systems represents a challenging task because of the wide range of the regimes covered by the flow. In fact, depending on the upstream plasma conditions, the Kn number spans from values typical from the continuum and slip regime above the dome until transitional and even free molecular regime in the sub-divertor regions and inside the vacuum pumping ducts: to describe such a range of gas rarefaction, an approach that has been recognized to be extremely valid is the Direct Simulation Monte Carlo (DSMC) method [1]. DSMC is a robust and reliable tool that is able to circumvent the numerical solution of the Boltzmann equation by simulating group of model particles whose behavior statistically mimics the one of the real gas molecules and, at the same time, to simulate non-isothermal flows. For this reasons, it is extremely suited to model the complex sub-divertor structure: studies of the neutral gas flows in both ITER [2] and JET [3] sub-divertor areas have been successfully performed implementing DSMC using input data from a SOL plasma code, such as SOLPS or EDGE2D. So far, though, the coupling between a plasma code and DSMC has been straightforward, with the output information from the edge plasma code imposed on the DSMC algorithm as inlet boundary condition. This works extends the procedure to a full iterative, but still manual, coupling between the DSMC approach and the SOLPS code applied to the JET divertor: the goal is to arrive to a self-consistent solution that takes into account their mutual interaction in terms of neutral particle recirculation. Specifically, the SOLPS edge plasma model outputs the flux quantities towards the pumping side that are then used as influx boundary condition for the sub-divertor domain, modeled by the DSMC algorithm. Once the first round of calculation has been performed, the data containing the information of the neutral outflux towards the private flux region, output of the DSMC run, is in turn used by SOLPS as a neutral particle source for the next iteration. This goes on until a consistent solution is found, that enhances in a coherent way the mutual influence between the two subsystems. Four plasma scenarios have been chosen for the purpose, and for each of them two round of iterations were enough to achieve convergence. A sensitivity analysis of the cryopump capture coefficient on the neutral particle reflux is performed as well, in order to understand how the pumping efficiency affects the flow pattern in the sub-divertor region. Results of the numerical simulations are presented in form of recirculation rates and contour plot of all the quantities of physical interest.

2. Divertor Configuration

The geometry used for the calculation represents a 2D cut of the 3D model for the JET Octant n.8. and it is depicted in Fig.1 (left). The original geometry foresees also the vertical lower port and the pipes leading to the barathron pressure gauge; previous simulations of this very same configuration [3], however, showed that the flow field in the latter region does not have a relevant influence for the flow field of the above sub-divertor and, for this reason, it has been neglected during the definition of the computational domain. The other main assumption that has been made is to consider a 2D model periodic in the z-direction, in order to considerably speed up the computational time. Although the configuration has been simplified from the original CAD model, it still preserves the initial high degree of geometrical complexity including the divertor field coils, the radiation shielding (louvres), the baffles and the cryopump as well. It is considered that only neutral particles are allowed to enter the sub-divertor domain throughout two main inclined gaps located in the high field side (HFS) and low field side (LFS), and corresponding to the gaps respectively between divertor tile 3 and 4 and between divertor tile 6 and 7. Both gaps have a similar length, namely 0.08 m and 0.082 m. while the cryopump, located in the LFS, has an overall length of 0.35 m.

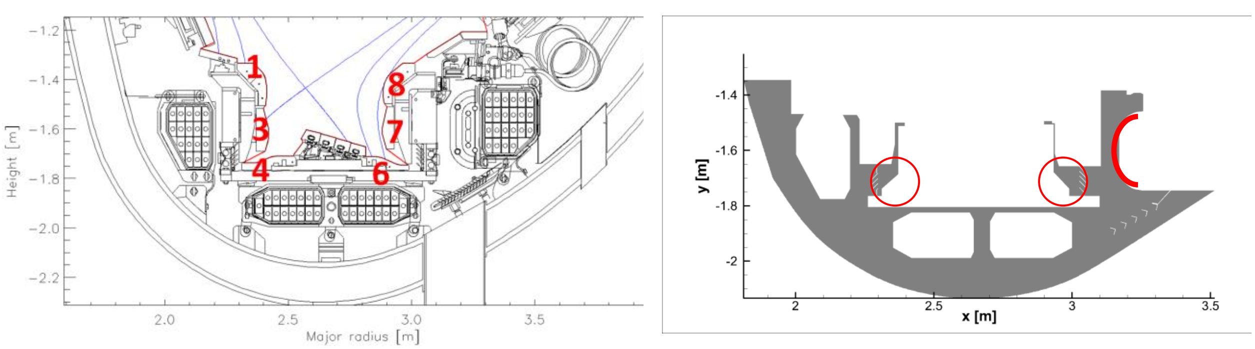


FIG. 1. 2D cut of the JET sub-divertor (left) and simplified geometry used in the DSMC simulation (right).

3. Numerical Modelling

The neutral flows in the sub-divertor area have been simulated using the DSMC algorithm based on the No-Time counter scheme [1]. Since DSMC has been proved a reliable method to describe the behaviour of rarefied gases, detailed descriptions of the method have been largely covered [1,4] and only the essential aspects of the implementation are here mentioned. Briefly, in a DSMC simulation, each model particle represents a large number of effective molecules (or atoms) in the physical system. At the beginning of the calculation, the computational flow domain is divided into a grid of cells and each model particle is assigned with initial position and velocity vectors. The flow then evolves in a series of time steps, each of duration Δt, in which free motion of the parcels is decoupled from their intermolecular collisions in the following way:

- First, free motion of particles is performed, estimating the new particle coordinates $r_{i,new}$ via the old ones $r_{i,old}$ as

$$r_{i,new} = r_{i,old} + v_i \Delta t. \quad (1)$$

If a particle during the motion crosses a solid surface, then the purely diffuse gas–surface interaction is applied and the particle continues its motion with a new velocity during the rest of time interval Δt.

- Then, intermolecular collisions are simulated by calculating the number of potential collision partners in each cell and randomly choosing two particles, whose collision occurs if the following condition is fulfilled:

$$\frac{\sigma_T v_r}{(\sigma_T v_r)_{max}} > R_f \quad (2)$$

where v_r is the relative velocity of this pair, σ_T is the total collisions cross-section of the particle, $(\sigma_T v_r)_{max}$ is the maximum collision probability and R_f is a random number uniformly distributed over the interval (0,1). If the pair is accepted, their velocities are replaced by new values according to the variable hard sphere (VHS) interaction law [1], otherwise, the random choice goes on until the number of potential collisions has been reached.

- At the end of each time step, finally, sampling of the macroscopic properties (number density n, the bulk velocity u and the temperature T) is conducted in the following way:

$$n = \frac{N_p}{V_C} F_N, u = \frac{1}{N_p} \sum_{i=1}^{N_p} v_i \, , T = \frac{m}{3kN_p} \sum_{i=1}^{N_p} (v_i - u)^2, \quad (3)$$

The final values of these quantities are given by the average amount during all time intervals Δt. The choice of the time step is essential, because the fundamental criterion in DSMC says that it should always be a fraction of the mean collision time, in order to consistently take into account all the events affecting the motion of the model particles: this condition is satisfied for a $\Delta t = 1 \mu s$. For the same reason, the grid must be chosen so that the cell size is a fraction of the mean free path of the molecules; in all the cases taken into account, a structured rectangular grid is used, with an average number of cells of 2×10^4.

4. Boundary Conditions

Molecular deuterium enters the DSMC domain through the HFS and LFS gaps with a reference density n_0 and temperature T_0. The incoming gas is assumed to be at rest, i.e. the velocity distribution of each component follows a Maxwellian distribution. Taking advantage of this hypothesis, the influxes towards the sub-divertor, output from SOLPS, can be easily converted into number density through:

$$n_{0,HFS-LFS} = \frac{4\Gamma_{in,HFS-LFS}}{v_t}$$

Being $\Gamma_{in,HFS-LFS}$, the influx from both gaps and v_t the thermal velocity of the far-field distribution.

The water cooled louvres and the divertor field coils are assumed to be kept at a room temperature of 300 K, while the outer wall of the vacuum vessel is assumed to be 473 K. Whenever a particle hits a stationary wall, then purely diffuse reflection occurs, meaning that the particle is re-emitted by the wall with a Maxwellian distribution centered on the wall temperature. The cryopump has been simulated by means of a surface kept at a temperature of 80 K with a given capture coefficient ξ, i.e. the ratio of number of particles absorbed by the pump itself versus the number of particles hitting its surface: the choice of the right value of ξ is essential because of its influence on the flow field. The pumping speed of the pump in situ in the JET torus is 200 m^3/s [5]; knowing this information, the capture coefficient can be deduced as

$$\xi = \frac{S}{S_{id}} = \frac{S}{A_{inlet}\sqrt{\frac{R_0 T}{2\pi M}}}$$

Where S is the effective pumping speed, S_{id} is the ideal pumping speed, A_{inlet} the cross section/pumping area, T the temperature of the pump and R_0 and M the properties of the gas being pumped. In the case of JET, a capure coeffiecient of 0.15 has been calculated.

At the end of each plasma case simulation, the updated albedo coefficients towards the private flux region are computed as:

$$\alpha_{HFS-LFS} = \frac{\Gamma_{out,HFS-LFS}}{\Gamma_{in,HFS-LFS}}$$

being Γ_{out} the ouflux towards the private flux region from each gap.

5. Results and discussion

In this section, the results of the simulations of both the plasma side and the divertor side are presented in terms of recirculation rates and contour plot. An additional sensitivity study has been performed for what concerns the sub-divertor domain, in order to investigate the factors influencing the most the pumping operation and, consequently, the flow patterns.

5.1. Albedo coefficients for HFS and LFS

Two rounds of iterations between SOLPS and DSMC were necessary to consistently update the values of the albedo coefficients of the two communication gaps between SOL and sub-divertor. Fig. 2 shows the converged map towards the final results, which are presented in Table 1. In all the four considered plasma cases, the final recirculation rates show a discrepancy of ~ 5% with respect to the original ones assumed for the LFS gap, and of ~ 9% to the ones assumed for the HFS gap: while the original SOLPS calculations have assumed higher recirculation fluxes from the sub-divertor towards the edge plasma, the new coupled runs proved that the actual pumping efficiency is, although slightly, better, i.e. the outfluxes towards the edge plasma are lower. Reasonably, the DSMC simulations resulted as well in values of the coefficients related to the LFS gaps that are lower that the ones for the HFS, due to the intrinsic asymmetrical position of the cryopump, directly facing the LFS gap. Since each gap presents the same trend in terms of albedos for all four considered cases, the updated values that could be considered in future simulations would be:

- α_{HFS} = 0.90 (previous one = 0.98)
- α_{LFS} = 0.85 (previous one = 0.90).

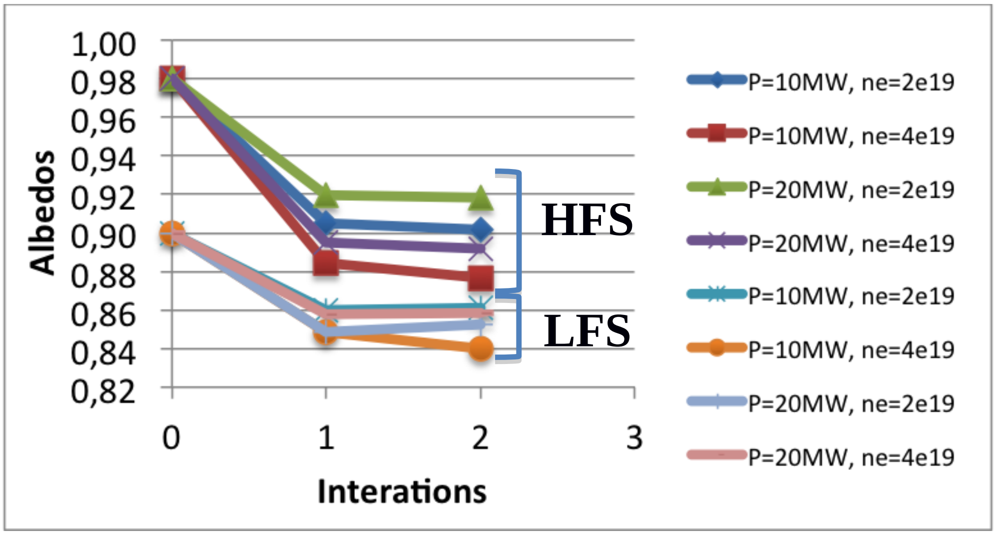
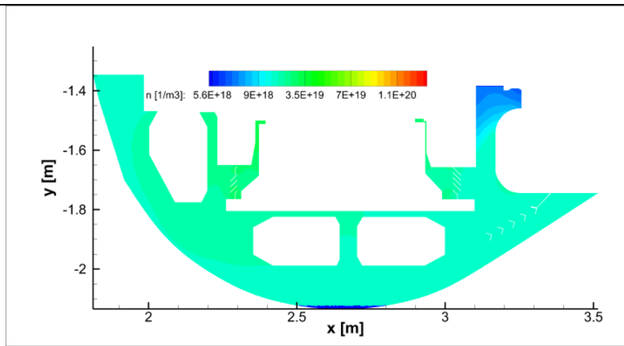


FIG. 2: Converged map for albedo coefficients

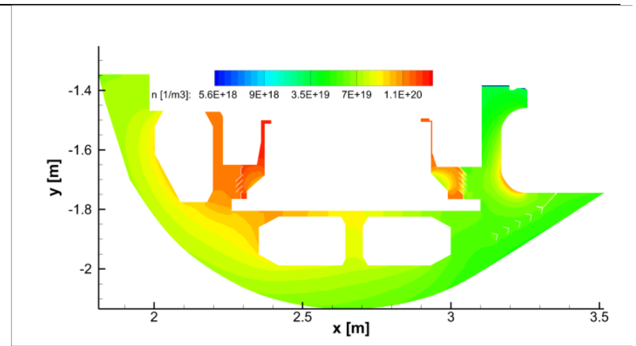
TABLE 1: UPDATED VALUES FOR ALBEDO COEFFICIENTS FOR HFS AND LFS GAPS.

	HFS Gap	LFS Gap
P = 10 MW, n_e = 2.0 x10^{19}	*0,90*	*0,86*
P = 10 MW, n_e = 4.0 x10^{19}	*0,88*	*0,84*
P = 20 MW, n_e = 2.0 x10^{19}	*0,92*	*0,85*
P = 20 MW, n_e = 4.0 x10^{19}	*0,89*	*0,86*
Average coefficient	**0,90**	**0,85**

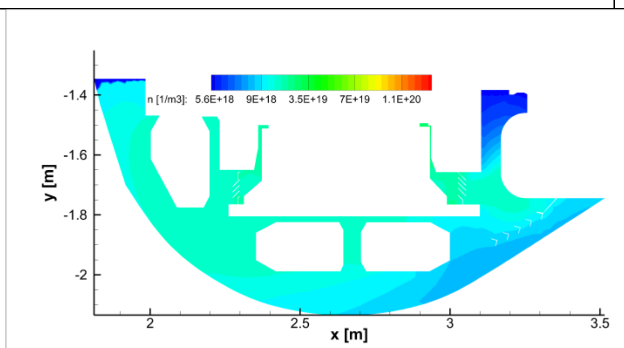
Contours of D_2 sub-divertor number density are presented in Fig.3 for both the higher density and lower densities plasma scenarios. The plots clearly explain the high recirculation rates that occur through the gaps: the incoming fluxes from the divertor hit the shielding louvres and remain confined in close proximity of the inlet, creating regions where the particle density is higher than in the rest of the structure and the gas particles themselves are reflected by the louvres towards the main chamber again.



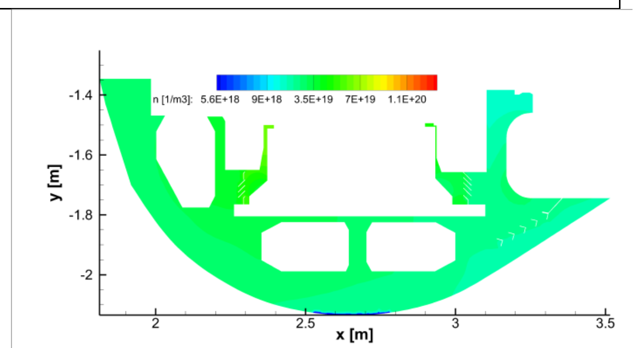
1: P = 10 MW, $\langle n_e \rangle = 2x10^{19}$



2: P = 10 MW, $\langle n_e \rangle = 4x10^{19}$



P = 20 MW, $\langle n_e \rangle = 2x10^{19}$



P = 20 MW, $\langle n_e \rangle = 4x10^{19}$

FIG. 3: D_2 number density contours from DSMC calculations for the four plasma scenarios.

5.1. Pumping efficiency studies

The impact on the pumping performance of different pumping and geometrical configurations in the sub-divertor area has been studied.

- For the plasma case correspondent to a power of 10 MW and a line-averaged electron density of $2x10^{19}$, a parametric study of the capture coefficient has been performed in order to assess the pumping efficiency of the cryopump in situ of the torus. Three additional, increasing values of ξ have been chosen (0.3, 0.6, 1) and the correspondent pumped particle flux has been computed; the latter has then been normalized with the total incoming particle flux, which is the sum of the influxes from both gaps, equal to $9.77x10^{21}$. Fig.4 (left) shows the results of the DSMC simulations: it can be seen that, even in the case of an ideal pump absorbing every particle hitting its surface, there is no relevant improvement in efficiency; in the best case scenario, only 16% of the sub-divertor incoming exhaust flux would be removed. The low sensitivity of the system to a dramatic increase in ξ could be due to the combined effect of the intrinsic asymmetrical position of the cryopump, located on the very LFS, and the presence of the field coils and water-cooled baffles, which significantly limit the conductance of the overall structure.

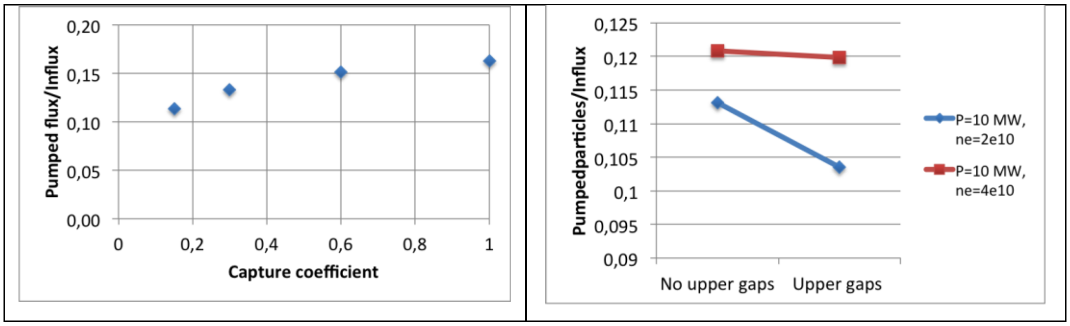
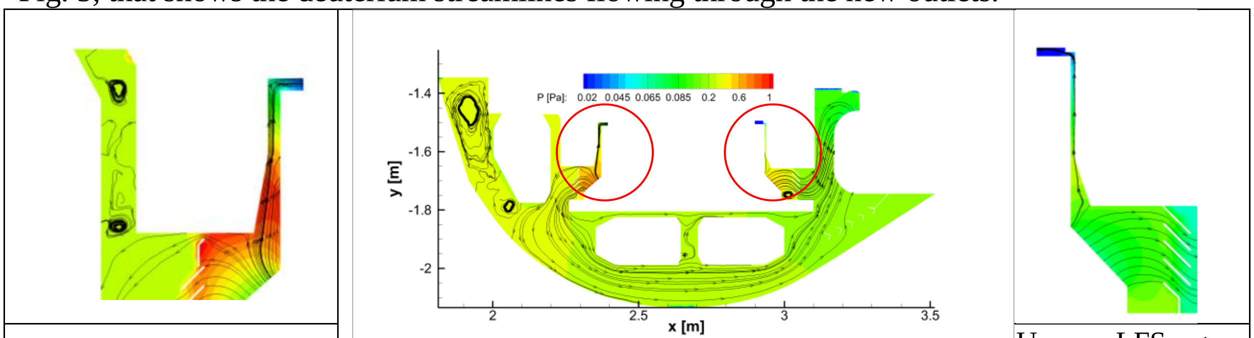


FIG. 4: Normalized pumped particle flux versus capture coefficient ξ (left) and in the case of open upper gaps (right)

- In order to quantitatively assess the entity of the recirculation rates towards the main chamber, two additional upper gaps, namely the upper gaps between tile 1 and 3 and between tile 7 and 8 (see Fig. 1 - left), have been considered as simply opened gaps, thus allowing D_2 to further recirculate back to the plasma side. Density contour plots of the converged results are found in Fig. 5, that shows the deuterium streamlines flowing through the new outlets.



Upper HFS gap (detail)

Upper LFS gap (detail)

FIG. 5: D2 Density contour plots with streamlines in the case of upper open gaps

Like in the previous study, as presented in Fig. 4 (right), in both plasma cases taken into account, the impact of the updated flow configuration does not significantly affect the flow field and the pumping efficiency: variation with respect to the nominal cases are within the 1% of the overall influxes. The reason of this result could be found in the geometrical feature of the gaps/outlet, whose smaller openings allow only a small fraction of the gas to escape, while the main flow pattern is still driven by the pump itself and by the main gaps.

6. Summary

The present work includes an integrated analysis of neutral deuterium gas dynamics in the JET divertor and sub-divertor. Two well known approach, the SOLPS code for the plasma side and the DSMC algorithm for the sub-divertor side have been manually coupled until convergence was reached in terms of neutral recirculation fluxes. Four JET divertor scenarios are studied, two with higher and two with lower electron density, and the calculations of the flow fields are shown. The pressure driven flows established in the divertor structure generate a high amount of particle exhaust flowing back towards the main chamber, with a rate that it has been found to differ from 5% to 9% to the original assumed values.

In continuation of this work, the DSMC algorithm could be further used to include gas mixtures (e.g. mixtures of He, D and D_2) and extended for 3D modeling, required to investigate the toroidal flow effects.

7. Acknowledgments

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