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. 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 user-defined, iterative procedure between SOLPS and DSMC has been established, using the neutral flux as the key communication term between the two codes. The goal is to understand and quantify in a self-consistent manner the mutual influence between the two regions, namely, how the particle exhaust pumping system controls the upstream plasma conditions. Parametric studies of the flow conditions in the sub-divertor, 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 [1] and the Direct Simulation Monte Carlo (DSMC) Method [2].

In the last few years, a lot of efforts [3-5] have been devoted to properly model the neutral gas 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 physics 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 Knudsen number Kn, defined as the ratio between the molecules mean free path and the characteristic length of the flow, spans a range from values typical of the continuum and slip flow 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 DSMC method.

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DSMC is a robust and reliable tool that is able to circumvent the numerical solution of the Boltzmann equation by simulating groups of model particles whose behavior statistically mimics that of the real gas molecules and, at the same time, to simulate non-isothermal flows. For these reasons, it is extremely suited to model the complex sub-divertor structure: studies of the neutral gas flows in both ITER [5] and JET [6] sub-divertor areas have been successfully performed with DSMC, using input data from a SOL plasma code, such as SOLPS or EDGE2D. So far, though, the coupling between plasma codes and the DSMC has been one way only, with the output information in terms of particle fluxes from the edge plasma code imposed on the DSMC algorithm as inlet boundary conditions.

This works extends the procedure to a full iterative coupling between the DSMC approach and the SOLPS code, which is then applied to the JET divertor. The goal is to arrive at 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 conditions for the sub-divertor domain, modeled by the DSMC code. Once the first iteration of calculation has been performed, the data containing the information of the neutral outflux towards the private flux region, which is the 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 takes into account in a coherent way the mutual influence between the two subsystems. Four plasma scenarios have been chosen for this purpose, and for each of them it was found that only two 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 the quantities of physical interest.

2. Divertor Configuration

The first main assumption that has been made is to consider a 2D model periodic in the z-direction (i.e. toroidal direction), in order to considerably speed up the computational time. A 2D cut of the 3D model for the JET Octant n.8. is depicted in Fig.1 (above) and the simplified geometry used for the calculation in Fig.1 (below); previous simulations of this very same configuration [6], including also the vertical lower port and the pipes leading to the pressure gauge, showed that the flow field in the latter region does not have a relevant influence in the upper sub-divertor area.

Although the configuration has been simplified from the original CAD model, it does still preserve the initial high degree of geometrical complexity including the divertor 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 through the two main inclined gaps located in the high field side (HFS) and low field side (LFS), and corresponding to the gaps between divertor tile 3 and 4 and between divertor tile 6 and 7, respectively. 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 0.40 m.

3. Boundary Conditions

Four SOLPS case studies have been selected [7], each corresponding to different JET plasma conditions in terms of higher and lower input power P and higher and lower line averaged electron density $\langle n_e \rangle_{l,edge}$, namely:

Case 1) P = 10 MW and $\langle n_e \rangle_{l,edge} = 2x10^{19}$

Case 2) P = 10 MW and $\langle n_e \rangle_{l,edge} = 4x10^{19}$

Case 3) P = 20 MW and $\langle n_e \rangle_{l,edge} = 2x10^{19}$

Case 4) P = 20 MW and $\langle n_e \rangle_{l,edge} = 4\text{x}10^{19}$

The different cases were chosen with the intention to understand the impact of different plasma upstream conditions on the flow pattern and on the pumping efficiency of the sub-divertor region. Molecular deuterium (viscosity index ω: 0.70) is assumed to leave the SOLPS domain and enter the DSMC one through the HFS and LFS gap, to which SOLPS associates each two albedo reflection coefficients, defined as the rate of reflected particles towards the plasma chamber, i.e. coming from the sub divertor, versus the rate of particles leaving the plasma chamber directed to the pumping side. SOLPS initally assumes the albedos to be 0.9 and 0.98 respectively for the LFS and HFS gap.

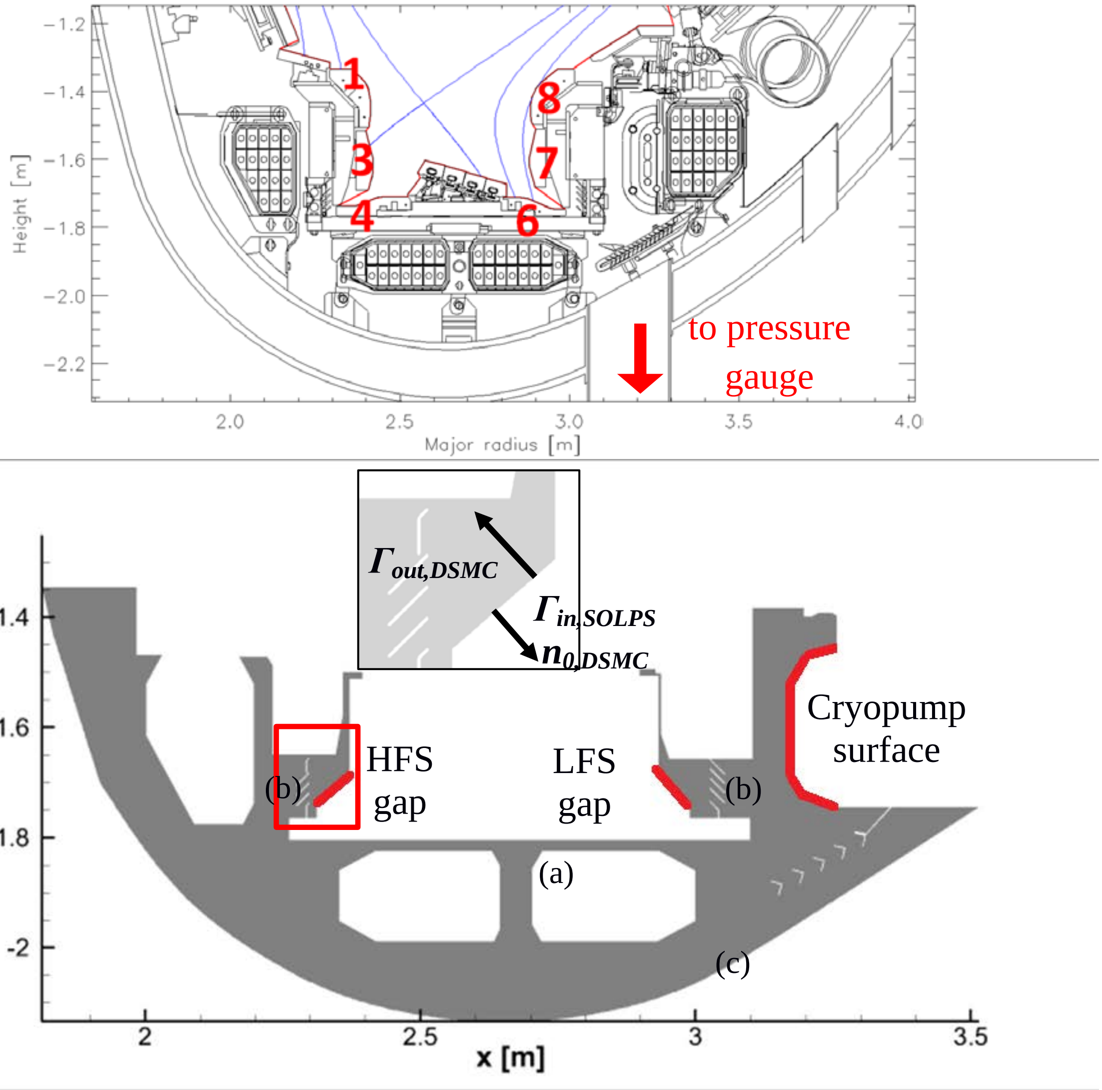


FIG. 1. 2D cut of the JET sub-divertor with divertor tiles numbering (above) and simplified geometry used in the DSMC simulation including: inlet gaps, cryopump, divertor coils (a), shielding baffles (b) and outer vessel surface (c)(below).

In each DSMC simulation, the gas crossing the gaps is assignend with a certain number density $n_{0,DSMC}$ and a temperature $T_{0,DSMC}$. As SOLPS assumed the far-field distribution of the gas leaving the plasma edge side to be at thermal equilibrium, so the DSMC algorithm assumes the incoming gas 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 from the gaps, output from SOLPS, can be easily converted into number density through:

$$n_{0,DSMC} = \frac{4\Gamma_{in,SOLPS}}{v_t}$$

Being $\Gamma_{in,SOLPS}$ the influx from each gap as shown in Fig. 1 (right) and v_t the thermal velocity of the far-field distribution. The DSMC input values for each plasma scenario are presented in Table 1.

TABLE 1: SUMMARY OF BOUNDARY CONDITIONS FOR DSMC CALCULATIONS.

		n_0 [1/m^3]	T [K]
HFS gap	P = 10 MW, $\langle n_e \rangle_{l,edge}$ = 2x10^{19}	1.41E+19	1620
	P = 10 MW, $\langle n_e \rangle_{l,edge}$ = 4x10^{19}	8.07E+19	1180
	P = 20 MW, $\langle n_e \rangle_{l,edge}$ = 2x10^{19}	7.30E+18	2295
	P = 20 MW, $\langle n_e \rangle_{l,edge}$ = 4x10^{19}	3.08E+19	1306
LFS gap	P = 10 MW, $\langle n_e \rangle_{l,edge}$ = 2x10^{19}	9.62E+18	2521
	P = 10 MW, $\langle n_e \rangle_{l,edge}$ = 4x10^{19}	6.00E+19	1302
	P = 20 MW, $\langle n_e \rangle_{l,edge}$ = 2x10^{19}	6.26E+18	4364
	P = 20 MW, $\langle n_e \rangle_{l,edge}$ = 4x10^{19}	1.81E+19	1970

The water cooled louvres and the divertor 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 at 473 K [8]. 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 [9]; 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 pumping speed, S_{id} is the ideal pumping speed, A_{inlet} the total toroidal pumping area (calculated A_{inlet}=8 m^2), T the temperature of the pump surface and R_0 and M the properties of the gas being pumped. In the case of JET, a capture coefficient of 0.15 has been calculated.

At the end of each DSMC simulation, the outflux Γ_{out} towards the private flux region from each gap is computed and the updated albedo coefficients are computed as:

$$\alpha_{HFS/LFS} = \frac{\Gamma_{out,DSMC}}{\Gamma_{in,SOLPS}}.$$

4. 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 have been largely covered [1], [11] and only the essential parameters of the simulations are here mentioned.

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 particles: for all the plasma scenarios considered above, this condition is satisfied for a Δt = 1 μs. 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, a structured rectangular grid is used, with an average cell size of 6 mm, resulting in an average number of cells of $2x10^4$. Finally, the ratio of real particles versus simulated one, known as F_N, ranged from 1 $x10^{11}$ to 1 $x10^{12}$, resulting in a total average number of simulated particles within the simulation domain of $20x10^6$.

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 plots. An additional sensitivity study has been performed for what concerns the sub-divertor domain, in order to investigate the factors influencing 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 reach converged values of the albedo coefficients of the two communication gaps between SOL and sub-divertor. Fig. 2 shows the convergence of the iterations 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 than those 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 SOLPS simulations are:

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

TABLE II: 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**

Another interesting consequence of this result is that it highlights an intrinsic inconsistency of the fluxes separately calculated by the two codes: although the discrepancies are confined, this clearly invalidates the initial assumption of gas at thermal equilibrium.

Contour plots of the two most representative cases are compared in Fig. 3. Results showed that the plasma parameter having the higher influence on the flow patterns is the electron density: in the low and high density case, the Kn number spans from 0.2 to 4, still remaining in the transitional, collisional flow range which is well described by DSMC. The D_2 density contour plots also clearly explains 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. The Kn number has been calculated in post-processing as the ratio between the mean free path and a length characteristic of the system, which in this case has been chosen to be an average between the two inlet gaps lengths, namely 0.81 m.

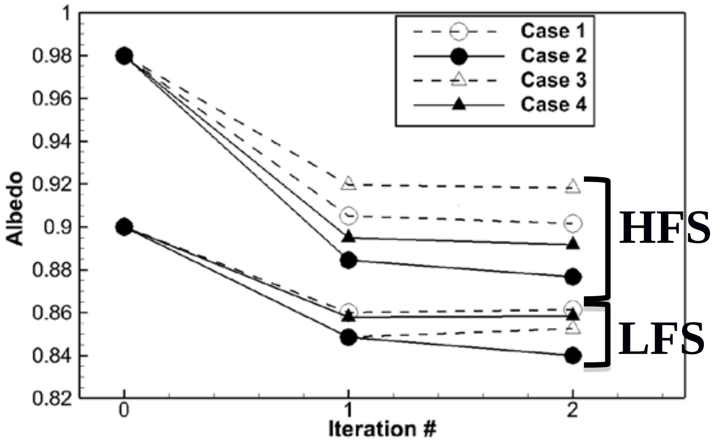
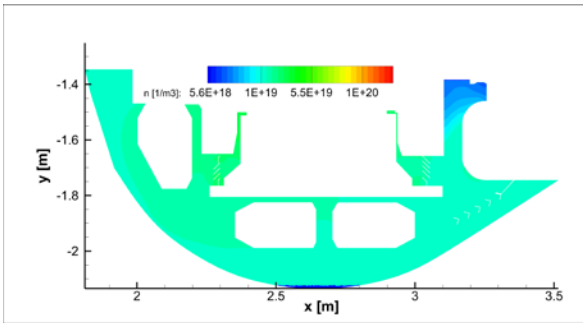
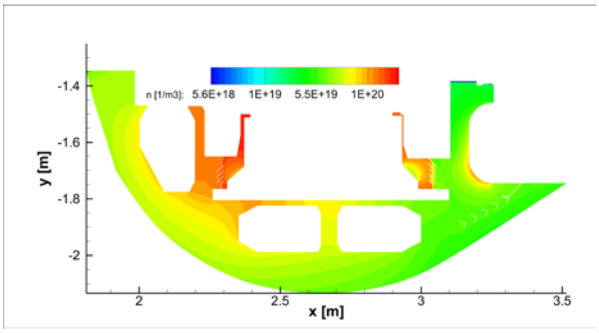


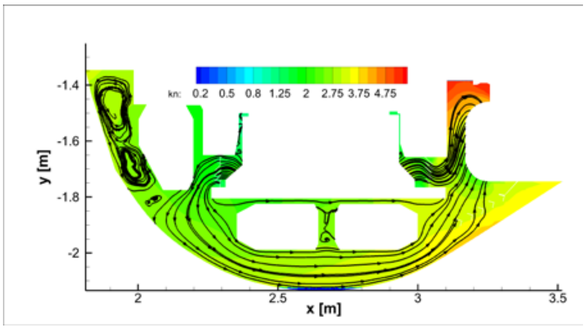
FIG. 2: Convergence of the albedo coefficients for the different considered plasma scenarios.



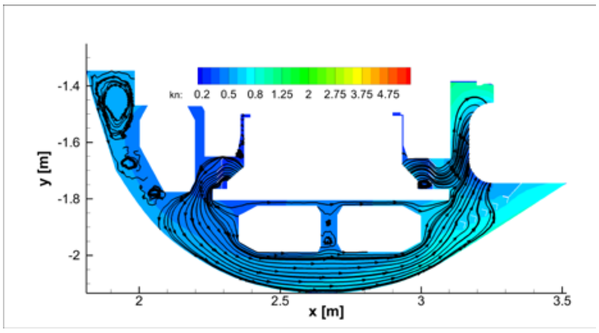
Case 1: P= 10 MW, $<n_e>_{l,edge} = 2x10^{19}$



Case 2: P = 10 MW, $<n_e>_{l,edge} = 4x10^{19}$



Case 1: P = 20 MW, $<n_e>_{l,edge} = 2x10^{19}$



Case 2: P = 20 MW, $<n_e>_{l,edge} = 4x10^{19}$

FIG. 3: D_2 number density (above) and Kn number – with streamlines towards the cryopump - (below) contours from DSMC calculations for Case 1 and Case 2.

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 1 (P = 10 MW, $<n_e>_{l,edge} = 2x10^{19}$), 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 corresponding 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 LFS, and the presence of the divertor coils and water-cooled baffles, which significantly limit the conductance of the overall structure.

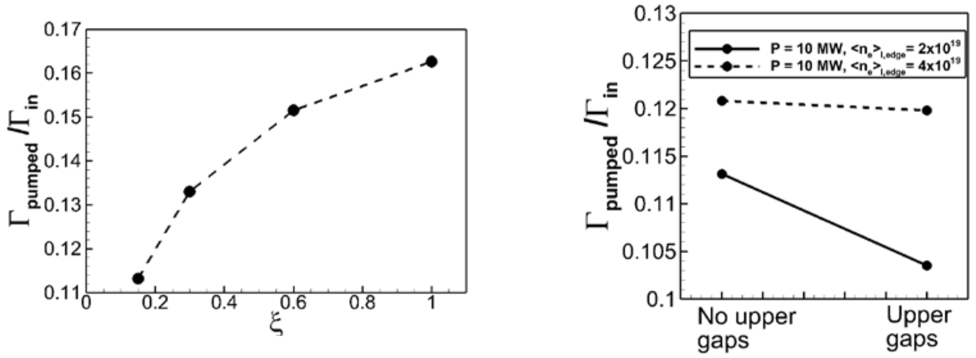


FIG. 4: Normalized pumped particle flux versus capture coefficient ξ (left) and in the case of open upper gaps (right).

- In order to present the influence of the geometrical inlet configuration on 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 open gaps, simply allowing D_2 to further recirculate back to the plasma side. Density contour plots of the converged results are found in Fig. 5, which shows the deuterium streamlines flowing through the new outlets.

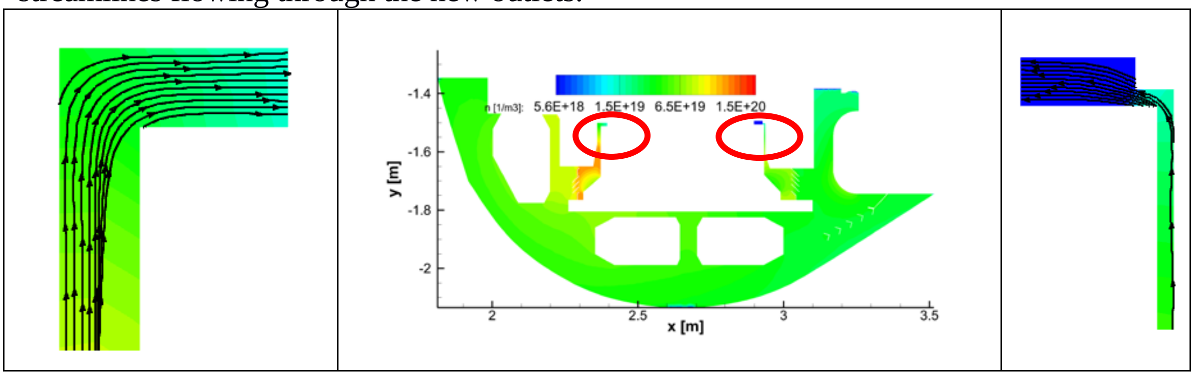


FIG. 5: D_2 Density contour plots in the case of upper open gaps and detail of streamlines flowing through the upper gap in the HFS (left) and LFS (right) for plasma case 2.

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 is 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 approaches, the SOLPS code for the plasma side and the DSMC algorithm for the sub-divertor side have been 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, each considering two different values of the input power, and the calculations of the D_2 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 was found to differ from 5% to 9% with respect to the assumed values in SOLPS standalone simulations.
In the future, 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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