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# Simulation of Neutral Gas Flow in the JET Sub-divertor and Comparison with Experimental Results

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**Abstract.** The present work presents a comparative study of the neutral gas dynamics in the JET sub-divertor. A complex model of the sub-divertor geometry is implemented and successful comparisons between corresponding numerical and experimental data have been performed. The experimental data represent the neutral gas pressure obtained by a sub-divertor pressure gauge. The recently developed Divertor Gas Simulator (DIVGAS) which is based on the Direct Simulation Monte Carlo (DSMC) method is applied. DIVGAS is able to predict the behaviour of the flow including macroscopic quantities of practical interest as for instance the pressure, temperature and bulk velocity. For all presented plasma cases, the deduced flow pattern is non-isothermal and covers the free molecular up to the transition flow regime. Furthermore, for low and medium divertor density simulations, recirculation effects occur through gaps between the vertical target tiles, which seem to be two order of magnitude less compared with the recycling ion flux onto the divertor walls. Finally, a direct comparison between DIVGAS and EIRENE code is conducted for the case of a simple benchmark problem, namely the gas flow through parallel plates and also for a more complex configuration, namely the gas flow through the JET sub-divertor. In the former case EIRENE underestimates the macroscopic quantities with relative difference of 5% as long as the Kn number remains equal or higher than unity. In the latter case a relative difference between 20-60% is mainly observed.

## 1. Introduction

Over the last few years much effort has been invested in modeling the neutral gas flow through the complex divertor and sub-divertor region in tokamak fusion reactors [1-4]. The main goal is the investigation of the impact of neutral gas dynamics on the particle removal process and the overall pumping efficiency during plasma operation. Neutral particle dynamics become more important when

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\* See the Appendix of F. Romanelli et al., *Proceedings of the 25<sup>th</sup> IAEA Fusion Energy Conference 2014, St. Petersburg, Russia.*

the plasma behavior is dominated by plasma-wall interactions (i.e. the recycling flux is greater than the deuterium injection by at least one order of magnitude) and/or when the operational regime is strongly dependent on the neutral behavior (e.g. within detached plasma scenarios or due to penetration of neutrals into the core etc.). Depending on the plasma conditions, the ratio of the mean free path to a characteristic length scale of the divertor, the so-called Knudsen number ( $Kn$ ), may vary over a wide range. This number in a fusion device covers values starting from the continuum ( $Kn \rightarrow 0$ ) and slip regime ( $10^{-3} \leq Kn < 0.1$ ) above the dome and close to the divertor targets and then, covers transitional regime ( $0.1 \leq Kn < 10$ ) and even free molecular ( $Kn \rightarrow \infty$ , collisionless) regime in the sub-divertor area and inside the vacuum pumps. Consequently, a reliable estimate of the macroscopic parameters in such a complex system requires a tool to describe the flow in the whole range of gas rarefaction. Currently, to calculate the plasma and neutral conditions in the SOL, the code package which is often used on fluid edge plasma modeling is the EDGE2D-EIRENE code [5], the EDGE2D consists of a 2D plasma fluid code, while the EIRENE algorithm [6] consists of a 3D Monte-Carlo solver for neutral-neutral interactions, based on the BGK kinetic model [7,8]. Over the years the EIRENE code has been proven to work sufficiently well in neutral modelling. However, no qualitative and quantitative comparison with a more complete neutral code has yet been performed in the sub-divertor region and under various operational plasma conditions. This statement comprises the motivation of this work. It is noted that the main drawback of the linear BGK approach is the inability to correctly describe simultaneously the transport coefficients of a specific neutral gas i.e. the gas viscosity and the thermal conductivity. Therefore, the BGK kinetic model is commonly applied only for pressure driven isothermal flows. To describe more efficiently non-isothermal flows (as expected in the sub-divertor region), the use of the Direct Simulation Monte Carlo method (DSMC) [9] is suggested in the present work.

The DSMC approach is based on a particle method, in which the solution of the Boltzmann kinetic equation is approximated by simulating groups of model particles that statistically mimic the behavior of real molecules. Investigations about neutral gas dynamics in the sub-divertor volume have been performed in [10-12] but all of them neglect the neutral-neutral collisions, which in the case of high densities play an important role for the flow field establishment. More recently, a similar investigation on the ITER sub-divertor was performed by successfully implementing the DSMC method coupled with SOLPS input data [13]. There, it was observed that high recirculation of neutrals behind the divertor targets occur (i.e neutral particles moving backwards to the plasma region). Following this applied workflow, the recently developed Divertor Gas Simulator (DIVGAS), which is a code based on the DSMC algorithm and is capable of modelling neutral gas flows in a tokamak sub-divertor, is applied for all the presented simulations.

The present work mainly focuses on the numerical simulation of the neutral gas flow and the calculation of overall quantities of practical interest i.e. pressure, density, temperature, bulk velocity, recirculation rates etc., inside the complex geometry of the JET sub-divertor by applying the DIVGAS code. For validation purposes, the numerical values are compared with existing JET ITER-Like Wall (ILW) [14] experimental data for the neutral gas pressure distribution in the sub-divertor region presented in [15]. The sub-divertor pressure measurements were obtained with a pressure gauge located at the end of the main vertical lower port of JET Octant 8 [16]. The comparison between experiments and numerical data is focused on different L-mode plasma scenarios, which cover low, medium and high neutral gas divertor densities, respectively. For each case, the corresponding EDGE2D-EIRENE plasma simulations have been performed. Then, the information about the neutral particles on the interfaces along the divertor geometry are extracted and imposed as boundary conditions (BC) for DIVGAS simulations. Following the above steps, the whole range of the Knudsen ( $Kn$ ) number is being covered and it made possible to quantify the differences between the numerical and experimental results in each regime. The last part of this work is focused on a direct comparison between DSMC algorithm and EDGE2D-EIRENE for the case of a simple flow configuration, namely gas flow through parallel plates [17] and for the case of a more complex JET sub-divertor geometry. The aim is to quantify the relative difference between both approaches for collisionless cases as well

as to exemplify the influence of intermolecular collisions and how they affect the macroscopic quantities across the flow field.

## 2. Divertor flow configuration

The scope of this work is to examine the 2D behavior of the molecular and atomic deuterium (i.e.  $D_2$  and  $D$ ) binary gas mixture flow inside the JET sub-divertor domain. Fig. 1 illustrates the used 2D-cut of the 3D JET CATIA model of the JET Octant No. 8. The cyan area highlighted in Fig. 1 was chosen as the simulation domain for the DIVGAS calculations. Although the selected geometry is simplified, it still preserves a high degree of complexity of the inner divertor structure, which limits the overall conductance of the system. In addition, the present configuration includes the cryopump and corresponding radiation shielding (louvres), the main lower port duct and the pipes, which connects the sub-divertor with the pressure gauge position (see Fig. 2a). This is necessary, because, as will be justified further below in this paper, due to the relatively high densities which are expected to appear there, the conductance cannot be easily calculated using available analytical solutions. The water cooled louvres and the divertor field coils are assumed to be maintained at room temperature i.e. 300 K, while the temperature of the vacuum vessel is assumed to be 473 K. The main assumptions on which the present study has been based mainly consist of the axisymmetry in the toroidal direction, the equilibrium of gas mixture (i.e.  $D$  and  $D_2$ ) before entering the sub-divertor area (i.e. assumption of gas at rest with zero incoming velocity), the absence of the volumetric/surface recombination and dissociation processes and finally the ideal constant pumping speed of the cryopump. Regarding the first assumption, although the authors are aware of the geometrical non-uniformity in the toroidal direction [16] (i.e. no symmetric gas puffing, existence of support structures and diagnostics), it was intentionally decided to take as first step an approach, which requires only modest computational efforts (i.e. 2D representation) but already includes some of the complex geometrical characteristics of such a flow domain. A complete 3D modelling, which additionally incorporates the study of the flow between the divertor cassettes, is foreseen as a future action once the feasibility of the present approach is demonstrated. Regarding the latter assumption of the pump modelling, it is noted that in all DIVGAS calculations an ideal pump was introduced where each particle that hits the surface of the pump is immediately absorbed. This corresponds to the upper limit case, in which the pump never saturates at maximum possible pumping speed.

## 3. Experimental setup

All the measurements which are presented in this work correspond to low confinement mode (L-mode) plasma cases with a JET ITER-like wall configuration [15]. The JET ITER-like wall (JET-ILW) consists of Be-coated inconel tiles [14], including bulk Be in high heat flux areas, such as limiters, and Be-coated carbon-fiber composite (CFC) surfaces in the other, recessed areas. The divertor plasma facing components (PFC) are made of bulk W for the horizontally inclined tiles at the low-field side (LFS) and W-coated CFC surfaces in all the other divertor areas, including the vertically inclined targets at both the high-field side (HFS) and LFS. More details about the experimental procedure and main machine parameters can be found in [15]. Furthermore, during the entire pulse series (i.e. JPN 81472-91), as the upstream separatrix density in the LFS mid-plane  $n_{e,sep,LFS-mp}$  increases, the response of the neutral gas pressure in the divertor is measured using a pressure gauge. It is noted that in order to reduce the influence of the stray magnetic field on the gauge, the pressure gauge system is located far downwards from the sub-divertor structure (almost 2.5 m away, see Fig. 2a). Both locations communicate through a series of pipes and bellows. The pressure system consists of two capacitance diaphragm gauges. The first device is a MKS 627D Baratron with pressure range of 0.1 Torr and accuracy in reading of 0.12%, while the second gauge is a Pfeiffer CMR 365 with 0.1 mbar pressure range and accuracy in reading of 0.5% [16]. It is noted that the latter device due to the low temporal resolution is only used as a cross reference for the former gauge. As a result, all the used pressure values presented here reflect only MKS 627D Baratron measured data.

## 4. Numerical modelling of the JET sub-divertor

### 4.1. The Direct Simulation Monte Carlo algorithm

The DSMC method, on which DIVGAS code is based, consists of a reliable and powerful numerical tool for modelling rarefied gas flows [17-19]. According to this method, a gas flow domain is divided into a network of cells. Initial positions and velocities of a large number of model particles are adopted. Each model particle in the simulation represents a large number of real molecules in the physical system. The motion of particles and their collisions are uncoupled by the repetition of the following steps:

- Free motion of particles is modelled, i.e. their new coordinates  $\mathbf{r}_{\text{new}}$  are estimated via the old ones  $\mathbf{r}_{\text{old}}$  as

$$\mathbf{r}_{\text{new}} = \mathbf{r}_{\text{old}} + \mathbf{v}\Delta t, \quad (1)$$

where  $\mathbf{v}$  is the vector of the molecular velocity. 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  $\Delta t$ .

- Intermolecular collisions are simulated following the Non-Time Counter method [5], i.e. the number of pairs to be tested in each cell is calculated as

$$N_{\text{coll}} = \frac{1}{2} N_p \bar{N}_p F_N (\sigma_T v_r)_{\text{max}} \frac{\Delta t}{V_C}, \quad (2)$$

where  $N_p$  is the number of particles in a cell at that moment,  $\bar{N}_p$  is the average number of particles in the same cell during all previous steps,  $F_N$  is the number of real particles represented by one model particle,  $\sigma_T$  is the total cross-section of the particle,  $v_{r,\text{max}}$  is the maximum relative velocity, and  $V_C$  is the cell volume. Two particles from the same cell are randomly chosen and they are accepted for collision under the condition  $\frac{v_r}{v_{r,\text{max}}} > R_f$ , where  $v_r$

is the relative velocity of this pair 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 [5]. As in the hard sphere model the collision cross section is given by the expression  $\sigma_T = \pi d^2$ , but now the molecular diameter  $d$  is a function of relative speed  $v_r$ , defined as

$$d = d_{\text{ref}} \left[ \left\{ \frac{2kT_{\text{ref}}}{m_r v_r^2} \right\}^{\omega - \frac{1}{2}} / \Gamma\left(\frac{5}{2} - \omega\right) \right]^{1/2}, \quad (3)$$

where  $d_{\text{ref}}$  is the average molecular diameter in a gas at the reference temperature  $T_{\text{ref}}$ ,  $m_r$  is the reduced mass of the gas, which is defined as

$$m_r = m_1 m_2 / (m_1 + m_2), \quad (4)$$

$\Gamma$  is the Gamma function and the parameter  $\omega$  is the viscosity index, which characterizes a given gas. In the present work since molecular and atomic deuterium gases were considered, the viscosity index is chosen as  $\omega = 0.73$  and  $\omega = 0.68$  respectively.

- Sampling of the macroscopic properties is conducted, i.e. the macroscopic quantities are calculated. The number density  $n$ , the bulk velocity vector  $\mathbf{u}$  and the temperature  $T$  in a computational cell are estimated by the following expressions

$$n = \frac{N_p}{V_C} F_N, \mathbf{u} = \frac{1}{N_p} \sum_{i=1}^{N_p} \mathbf{v}, T = \frac{m}{3kN_p} \sum_{i=1}^{N_p} (\mathbf{v} - \mathbf{u})^2, \quad (5)$$

respectively. The final values of these quantities are given by the average amount during all time intervals  $\Delta t$ .

In the above framework, an unstructured computational grid, which consists of  $5 \times 10^4$  triangular cells, was applied in the computational field (Fig. 2b). In all the present simulations an optimum value of  $\Delta t = 0.1 \mu\text{s}$  has been used, which takes into account the fundamental criterion of DSMC that  $\Delta t$  should be a fraction of the mean collision time. On the other hand, the average number of particles in each cell of the flow field was ranging around 50 particles per cell. This number assures that the

statistical scattering of macroscopic quantities along the computation domain is sufficiently low. All the above parameters were chosen to maintain the accuracy of the calculated results within two significant digits. In addition, the Larsen–Borgnakke model [20], which describes the energy exchange between translational and internal degrees of freedom during binary collisions of diatomic molecular deuterium among the gas mixture, is considered. Furthermore, the particle-wall interactions are assumed to be purely diffuse, namely the reemitted particles forget their previous information and are reflected back to the flow domain with a Maxwellian distribution function based on the wall temperature. It is noted that, in the present algorithm the recombination and dissociation processes are not taken into account and therefore, when a  $D_2$  molecule or a D atom hits a wall surface, it remains as a molecule or as an atom respectively. The DIVGAS code used in the present work has been implemented in OpenFOAM [21], an open-source C++ toolbox for computational fluid dynamics. This solver, which is called dsmcFoam, has been rigorously validated for a variety of benchmark cases [22] and it has been modified accordingly for the purpose of the present work. The present DIVGAS code is fully parallelized and for all the presented calculations a high-performance computer named “bwUniCluster” was used, by utilizing up to 128 cores for each case.

#### 4.2. EDGE2D-EIRENE simulations

The scrape-off layer in attached, partially detached and fully detached divertor plasmas obtained at the low field side (LFS) divertor target were previously simulated using the edge fluid code EDGE2D-EIRENE [5,6] as described in Ref. [15]. The experimental data and EDGE2D-EIRENE predictions shown throughout this publication are entirely based on the work presented in [15]. The magnetic configuration corresponds to a low upper-triangularly ( $\delta \sim 0.2$ ) with the high field side (HFS) strike point on the vertical target and the LFS strike point on the horizontal target. In the simulations the electron density at the upstream separatrix was varied by deuterium gas fuelling from the top and the divertor (private flux) regions. Consequently, low-density ( $1 \times 10^{19} \text{ m}^{-3}$ ), high-temperature (40 eV) divertor plasmas at the LFS divertor target were obtained at low upstream electron density ( $8 \times 10^{18} \text{ m}^{-3}$ ), and high-density ( $3 \times 10^{20} \text{ m}^{-3}$ ) and low-temperature (3 eV) at intermediate densities ( $1.5 \times 10^{19} \text{ m}^{-3}$ ) at the onset of detachment (figure 11 of Ref. [15]). The predicted ion and power fluxes to, and the electron temperatures at the LFS target are consistent within a factor of 2 of the measured parameters for these upstream electron densities. Reduced electron densities ( $< 1.0 \times 10^{19} \text{ m}^{-3}$ ) and sub-eV electron temperatures were predicted for the highest upstream electron densities ( $> 2.0 \times 10^{19} \text{ m}^{-3}$ ). The predicted low temperature conditions at the LFS divertor plate are consistent with line ratio analyses of line-integrated, high-n deuterium Balmer emission [23]. However, measurements of the total radiated power (Fig. 11b and d of Ref. 15) and the line-integrated deuterium emission of low-n Balmer lines [24] showed a radiation shortfall, which could potentially be due to significant differences in the actual and predicted neutral distribution in the divertor. In addition, significantly higher electron densities are inferred from Stark broadening analyses of line-integrated high-n deuterium Balmer lines across the divertor plasma compared to low electron densities at the LFS divertor plate. In contrast, EDGE2D-EIRENE presently predicts the electron densities to peak at the plate. Addressing the latter two issues is beyond the scope of this publication. Here, the existing EDGE2D-EIRENE predictions as given in ref. [16] are taken as they stand, and the DIVGAS analyses presented here will be re-evaluated when these issues are resolved.

The Monte-Carlo neutrals code EIRENE [6] is used as inputs to predict the atomic and molecular deuterium fluxes to the divertor wall surfaces, including the neutral fluxes representing the pumping plena on the HFS and LFS divertor corners (Fig. 2b). In these EDGE2D-EIRENE simulations, the sub-divertor structure is not included, and the neutral fluxes into the sub-divertor are determined by the albedos of the assumed pumping plena. Here, the divertor corners are assumed pumping at 6% of the incoming atomic and molecular fluxes. In addition, EIRENE provides the neutral fluxes to by-pass leaks between toroidal gaps along the vertical targets (Fig. 2a) assuming zero pumping across these gaps.

## 5. Results and discussion

In this section, the results obtained from the DIVGAS calculations and their comparison with corresponding experimental results from the pressure gauge are presented for different plasma collisionality cases. An investigation of neutral gas dynamics, which consist of a parametric analysis of the flow field based on macroscopic parameters of practical interest, is conducted. Furthermore, a direct comparison between DIVGAS and EIRENE is performed for two cases, namely (i) the case of deuterium gas flow through parallel plates and expansion into vacuum for discussing principle aspects of the two approaches, and (ii) the more complex geometrical configuration as the one presented in Fig. 2a. The main objectives are firstly the estimation of the relative difference between the macroscopic parameters of both numerical approaches along the flow field and secondly the quantification of the influence of intermolecular interactions in the estimated values for the given plasma conditions.

### 5.1. Neutral gas dynamics in the JET sub-divertor

In Fig. 3a, the comparison between the calculated DIVGAS and measured pressure at the gauge location, as a function of the upstream electron density at the LFS mid-plane  $n_{e,sep,LFS-mp}$  is presented. As described in [15], by increasing  $n_{e,sep,LFS-mp}$ , the pressure at the gauge location increases exponentially over two decades. A similar behaviour is reproduced by the DIVGAS results. A no more than a factor of two difference between numerical and experimental data is found. Taking into account all the assumptions and simplifications described in Section 2, it is clearly demonstrated that the DIVGAS code is able to describe the flow conditions of neutral gases even in such complex geometries. In Fig. 3b, the experimental maximum electron density in the LFS divertor target and the sub-divertor pressure versus the separatrix upstream plasma density is presented. It is clearly seen that the outer divertor target density drops at the highest upstream density and so does the sub-divertor pressure. When the plasma is fully detached, the pressure in the divertor region (and this sub-divertor) decreases, as a result of the low divertor plasma temperature, which allows neutrals to move towards the installed cryopump. The scaling of the sub-divertor pressure with the upstream plasma density includes all the plasma physics from the outer midplane to the divertor, which is still a complex issue to address.

For a better understanding of the neutral gas dynamics in the area of the sub-divertor, a calculation of macroscopic quantities of practical interest in various locations (probes) along the flow domain has been performed. In Fig. 2b, the five representative locations, which cover a wide area of the sub-divertor, are depicted. For each of these points, the local neutral pressure and temperature of gas mixture and the corresponding local Kn number have been estimated. The local Kn number is defined as the ratio of the local mean free path, over a characteristic length of the flow, which is the height of the lower-LFS boundary condition interface, namely  $Kn = \lambda_{VHS}/H_{Lower-LFS}$ . The mean free path  $\lambda_{VHS}$  is obtained by the following expression,

$$\lambda_{VHS} = \left\{ \sqrt{2} \pi d_{ref}^2 n (T_{ref}/T)^{\omega-1/2} \right\}^{-1}, \quad (6)$$

where  $n$  and  $T$  is the local number density and temperature respectively. For the given geometry, the height of the lower-LFS interface is equal to  $H_{Lower-LFS} = 40$  mm. The choice of this dimension as characteristic length is mainly based on the fact that in all density cases the particle fluxes towards this surface are the highest of all the divertor and sub-divertor interfaces.

In Fig. 4a, the gas mixture temperature in the above-defined locations is presented predicting that the temperature in the sub-divertor area is almost independent of the plasma conditions and strongly depends on the defined temperature of the stationary walls. Moreover, the flow field is shown to be non-isothermal with the temperature to range from 300 to 450 K. In Fig.4b, the estimated Kn number in the five different locations in terms of the upstream density is presented. It indicates that for the case of low  $n_{e,sep,LFS-mp}$ , the Kn number is high and varies between  $10^2$  to  $10^3$ , which indicates that the flow is highly rarefied and belongs to the collisionless regime. On the other hand, as  $n_{e,sep,LFS-mp}$  increases, then the Kn number decreases almost two orders of magnitude until the transition

regime ( $Kn \sim 1$ ) is established. Then, the presence of the intermolecular interactions becomes an important factor for the prediction of the macroscopic quantities. In addition, it is noted that the Kn number especially in the location #2 for the low and medium density cases is always decreased due to the high incoming particle flux injected from the Lower-LFS gap. On the other hand in locations #3, #4 and #5 the Kn number remains almost constant for each case. The last finding explains the uniformity of the flow in this region. The same observation can be visualized in Fig.5a, where the pressure of the gas mixture (i.e D and D<sub>2</sub>) is presented. Since pressure is inverse proportional to the Kn number, it is deduced that the pressure variation along the flow field follows qualitatively this trend. Another significant observation in such a complex geometry is the difference between the measured pressure in the pressure gauge location and the calculated one in the sub-divertor area (location #3), shown in relative terms versus the upstream density in Fig. 5b. Based on this plot, it is deduced that as the divertor upstream density increases, the relative difference between the pressure gauge and #3 location decreases and lies between 20 to 35% for the case of the considered flow (i.e the pressure in location #3 is always higher than in the gauge location, for each gas species). Such a discrepancy is mainly introduced due to the overall conductance of the lower port duct and the pipes connecting the gauge. This strong effect is for the first time quantified in this paper and it is suggested to be used in the evaluation of future pressure measurements, or in the re-evaluation of previous data.

In Fig. 6, the estimated pressure inside the divertor region in terms of the pumped particle flux is presented and the linear dependence between the two quantities is clearly illustrated. The constant slope of the line, which connects all the presented points, corresponds to the effective pumping speed  $S_{eff}$  of the cryopump which is deduced to be 75.5 m<sup>3</sup>/s/m and corresponds to the assumption of an ideal pump with capture coefficient  $c$  equal to unity. Approximating the total circumference length of the cryopump to be 20 m [25], then the total pumping speed is equal to 1510 m<sup>3</sup>/s, which is 7.5 times higher than the measured pumping speed of 200 m<sup>3</sup>/s (for D<sub>2</sub>) as given in [25]. Although such a discrepancy in the assumed boundary conditions exists, the influence of the pumping speed on the measured pressure in the gauge location is believed to be negligible. This can be justified due to the very small conductance of the connecting pipes, which are located below the lower port duct towards the pressure gauge. Specifically, if free molecular conditions are assumed, then the overall conductance of the connecting pipes is deduced to be more than four orders of magnitude lower than the above pumping speed of 1510 m<sup>3</sup>/s. Moreover, based on the above calculated ideal pumping speed, the corresponding capture coefficient of the cryopump may be derived. By using the equation  $S = c \times S_{ideal}$ , where  $S$  is the actual pumping speed,  $c$  is the capture coefficient with  $0 \leq c \leq 1$  [26] and  $S_{ideal}$  the ideal pumping speed of a cryopump, the deduced capture coefficient (i.e the efficiency of the pump) for a cryopump with actual pumping speed equal to  $S = 200$  m<sup>3</sup>/s [25] and ideal pumping speed equal to  $S_{ideal} = 1510$  m<sup>3</sup>/s, is  $c = 0.132$  for D<sub>2</sub>. Such a value seems to be a reasonable estimation, which characterizes the vacuum technological design of a cryopump [26]. To the best of the authors' knowledge, there is not any available experimental characterization of the JET cryopump in the literature and therefore the benchmarking of the above capture coefficient value is not possible. On the other hand, the above concept of estimating the capture coefficient of any pump is straightforward and can be further applied for the optimization of any tokamak vacuum system.

Finally, an important qualitative observation regarding the behaviour of the flow field depending on the operational upstream conditions is the recirculation of neutrals, which takes place through the inlet boundaries for all the upstream plasma densities examined in this work. In Fig. 7a, the gas mixture streamlines for the case of low-density case is presented and it is seen that only in the Lower-HFS gap gas mixture is going towards the plasma chamber (see the direction of streamlines). The particle flux, which flows towards the plasma region, is equal to  $1.7 \times 10^{18}$  (s<sup>-1</sup>m<sup>-1</sup>). In the case of medium density case, recirculation of neutral gas mixture takes place in the Lower-HFS and in the Upper-LFS gap as shown in Fig. 7b, with the particle flux to be equal to  $8.4 \times 10^{18}$  (s<sup>-1</sup>m<sup>-1</sup>) and  $1.3 \times 10^{19}$  (s<sup>-1</sup>m<sup>-1</sup>) respectively. On the other hand, for the high-density case (Fig. 7c) recirculation of gas mixture takes place only in the Upper-LFS gap behind the divertor vertical targets. The calculated particle flux for that case is equal to  $4 \times 10^{19}$  (s<sup>-1</sup>m<sup>-1</sup>). It is noted that for all the above cases the neutral

recirculation behind the divertor tiles is two or even three orders of magnitude lower than the ion recycling flux to the walls and therefore the influence of neutral particles on the overall divertor particle balance is assumed to be negligible. On the other hand, it is necessary to be considered that for the case of even higher divertor densities, the recirculation neutral particle fluxes might not be as low as the ones currently presented and therefore special attention should be given in taking into account such contribution on the divertor plasma edge modelling.

## 5.2. Direct comparison between DSMC and EDGE2D-EIRENE

In Fig.7, a direct comparison between the two numerical approaches is conducted for the case of a simple flow configuration, namely, gas flow through parallel plates with length to height ratio  $L/H=5$  and expansion into vacuum. More specific, this flow problem has been extensively investigated in [17] by the DSMC in the whole range of the Kn number and it is assumed as a benchmark problem in the field of vacuum gas dynamics [27]. The details of the flow configuration and the numerical scheme are omitted here and only representative flow cases will be used for comparison purposes. The aim is to compare macroscopic quantities as the pressure and the temperature along the symmetry axis of the flow domain and to quantify the differences in each region. It is noted that although the EIRENE code is able to introduce intermolecular collisions in the neutral simulations, in the present EIRENE version this option was switched off. Therefore for consistency purposes the direct comparison will be limited only in the collisionless regime. The corresponding DSMC collisional results will be recalled in order to quantify the influence of intermolecular interactions on the corresponding macroscopic flow quantities. In Fig. 8a, the dimensionless pressure profile along the symmetry axis  $y = 0$  is depicted. It is seen that for the case of  $Kn \rightarrow \infty$ , collisionless EIRENE underestimates the calculated pressure. The relative difference is constant and has the order of 5% along the whole symmetry axis. In addition, it is seen that by reducing the Kn number to  $Kn = 1$ , the pressure profile does not significantly change. Further decrease of the Kn number, i.e.  $Kn = 10^{-2}$ , towards the viscous regime, influences drastically the profile pattern since the pressure drop becomes non-linear inside the parallel plates. These calculations, thus indicate that the collisionless EIRENE version is capable of producing reliable results within the range of free molecular and transition flow regimes, while for a case between transition and viscous flow regime, the presence of intermolecular collisions dominates in the estimation of the macroscopic parameters and therefore only the collisional EIRENE version should be applied. In the same sense, Fig. 8b, represents the dimensionless temperature profile along the symmetry axis  $y = 0$ . Also in this case, the collisionless EIRENE version underestimates the temperature especially in the outlet region, downstream of the parallel plates and the relative difference remains at the same level as before and is of the order of 5%. Similar conclusions regarding the influence of neutral particle interactions can be extracted.

In the above framework of the direct comparison between the two algorithms, it is of high interest, to extend it towards a more complex configuration and to perform a similar study on the obtained differences. Thus, in Fig. 9, the percentage difference between DIVGAS and collisionless EIRENE is presented for the case of molecular deuterium number density (Fig. 9a) and temperature (Fig. 9b) based on the complex geometry of Fig. 2. The results presented correspond to the highest value of the upstream density, equal to  $n_{e,sep,LFS-mp} = 1.1 \times 10^{19} (\text{m}^{-3})$ . It is seen that for the case of the number density, the collisionless EIRENE code preserves the same behaviour of underestimating the macroscopic quantity of about 30% in the whole flow domain. Moreover, for the case of temperature, on one hand, both algorithms coincide quite well in the lower port region as well as the piping network of the sub-divertor, where no large temperature gradients occur. On the other hand, close to the cryopump a relative difference between 20-60% is observed, since the flow field in that region is mainly characterized by large temperature gradients due to inserting particles and the different wall temperatures. Finally, it is noted that the same behaviour has been observed for cases with lower upstream separatrix density. Here it should be noted that the present comparison between DIVGAS and EIRENE codes is a first step for quantifying the differences between two approaches and this

work will be definitely extended in an even more detailed comparison by taking as well into account the intermolecular interactions.

## 6. Summary

The present work includes a comparative study of the neutral gas dynamics in the JET sub-divertor. A realistic 2D (poloidal) model of the sub-divertor geometry is applied. The experimental data represent the neutral gas pressure obtained by the pressure gauge (which is located  $\sim 2.5$  m below the cryopump) for an L-mode plasma case. The DIVGAS code is able to quantitatively predict the behaviour of the flow domain including macroscopic quantities of practical interest as the pressure and temperature and bulk velocity. The numerical pressures in the sub-divertor area differ by a factor of two within the corresponding experimental values. For all the presented plasma cases, the deduced flow pattern is non-isothermal and a factor of two relative difference of temperature distribution for different plasma conditions is obtained. The relative difference between the measured neutral pressure at the pressure gauge location and the pressure in a representative sub-divertor location varies between 20-35 % depending on the upstream plasma conditions. Furthermore, for low, medium and high upstream density simulations, recirculation of neutrals occurs through the gaps between the target tiles. The recirculation particle flux for these cases is assumed to be negligible compared with the recycling ion flux on the walls. However, the influence of neutral recirculation on divertor plasma conditions is expected to be more significant for higher collisionality divertor conditions. In addition, a direct comparison between DIVGAS and the collisionless EIRENE code is performed based on a classical benchmark and a more complex geometrical configuration. The comparative study for the former case shows that the discrepancy between both codes is about 5% in the calculation of macroscopic quantities i.e. pressure, number density and temperature as long as the Knudsen number is higher than unity, while for the latter case varies between 20% in the free molecular flow regime and 60% in the transitional flow regime. For lower Kn values (i.e. viscous flow regime) the presence of intermolecular collisions dominates the estimation of any macroscopic quantity of practical interest and therefore in this case the collisionless EIRENE code provides underestimated values.

The value of the presented workflow of modelling the JET sub-divertor is based mainly on the fact that the DIVGAS code is benchmarked under a known geometrical structure and it can be further exploited in the design and optimisation of the DEMO and JT-60SA divertors, in which it is expected that higher densities (i.e. low Knudsen numbers) will be present. Therefore, a correct description of the neutral intermolecular interactions should be greatly considered. Additionally, the DIVGAS code is proven to be the right tool for the understanding of the particle exhaust system and the role of pumping as plasma actuator in a tokamak. Finally, the DIVGAS code can be further applied as benchmark tool for any new proposed algorithm, which includes neutral particle interactions.

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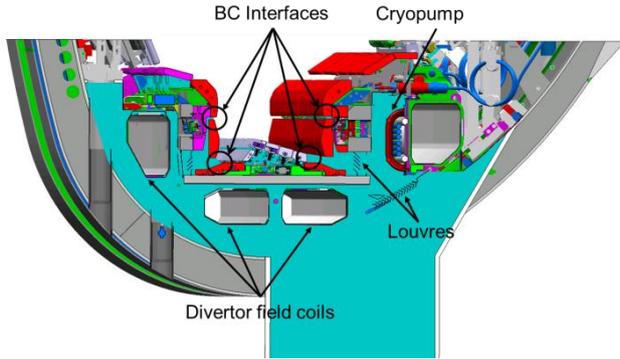


Figure 1: Geometrical representation of sub-divertor structure.

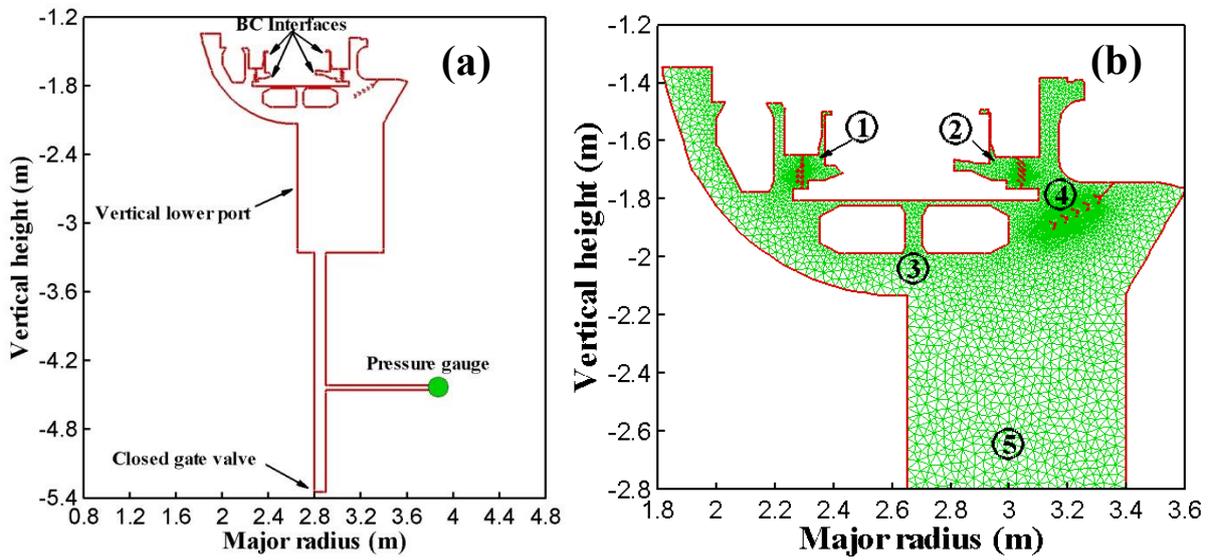


Figure 2: (a) 2D model of the JET sub-divertor. (b) Various locations (probes) in the sub-divertor area.

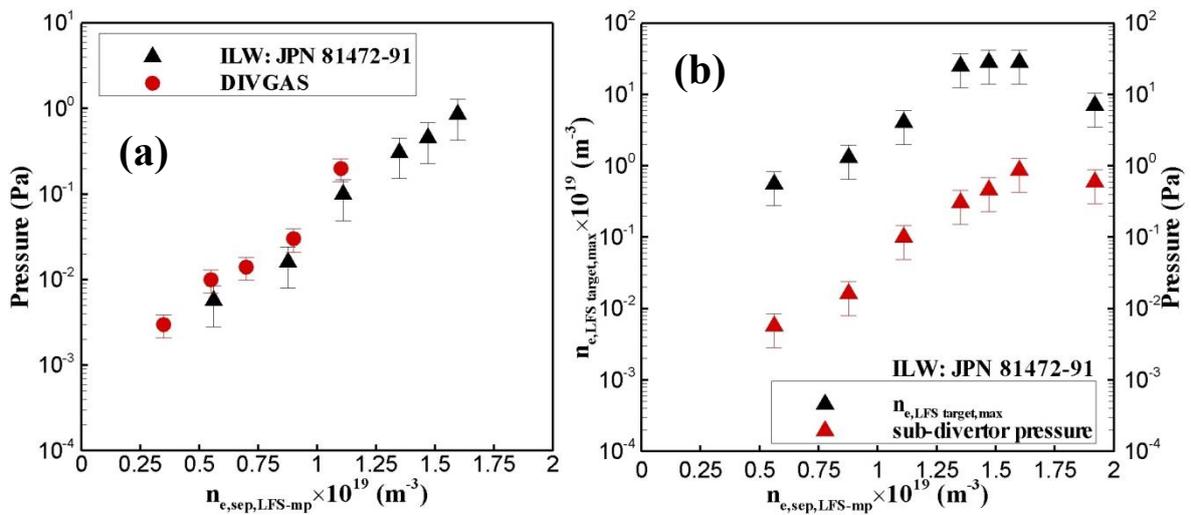
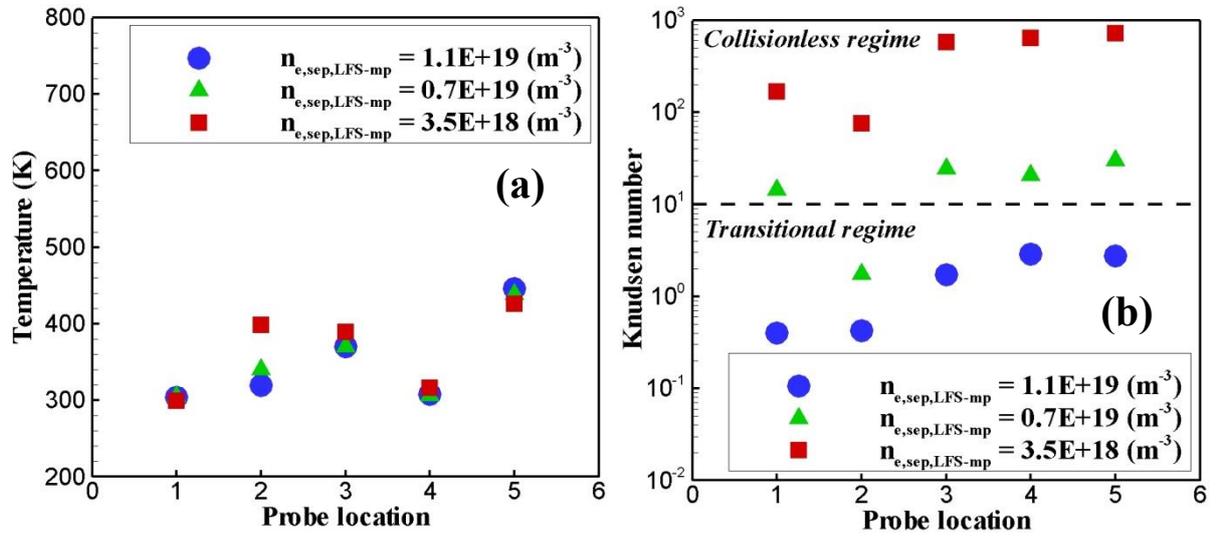
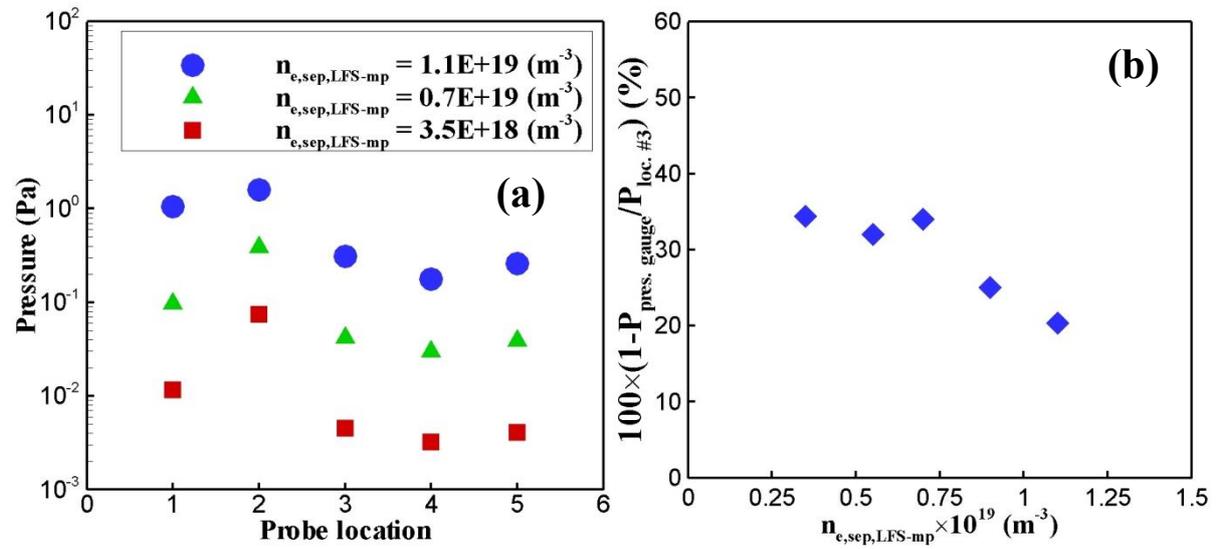


Figure 3: (a) Comparison between the DIVGAS and experimental molecular deuterium pressure in the location of the pressure gauge. (b) The experimental maximum electron density in the LFS divertor target and the sub-divertor pressure versus the separatrix upstream plasma density.



**Figure 4:** (a) Overall temperature and (b) the local Kn number for the gas mixture in various locations of the sub-divertor.



**Figure 5:** (a) Pressure for gas mixture in various locations of the sub-divertor. (b) Relative difference between the pressure at the gauge and the pressure at location #3 in the lower middle part of sub-divertor.

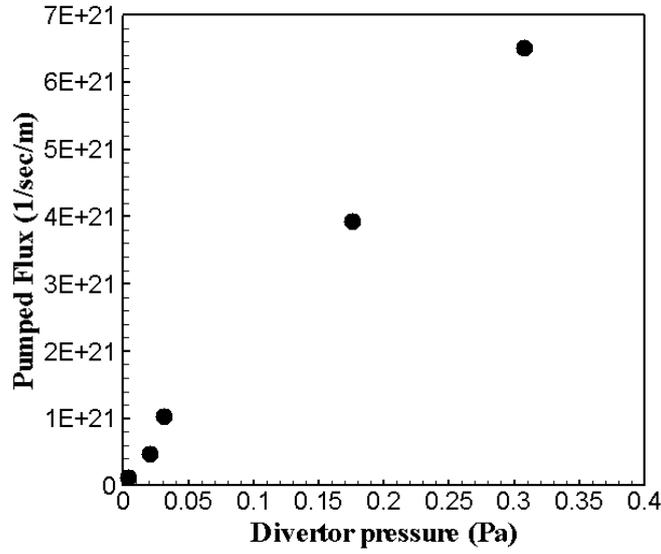


Figure 6: Calculated pressure in the divertor (pressure at location #3) in terms of the pumped gas mixture flux.

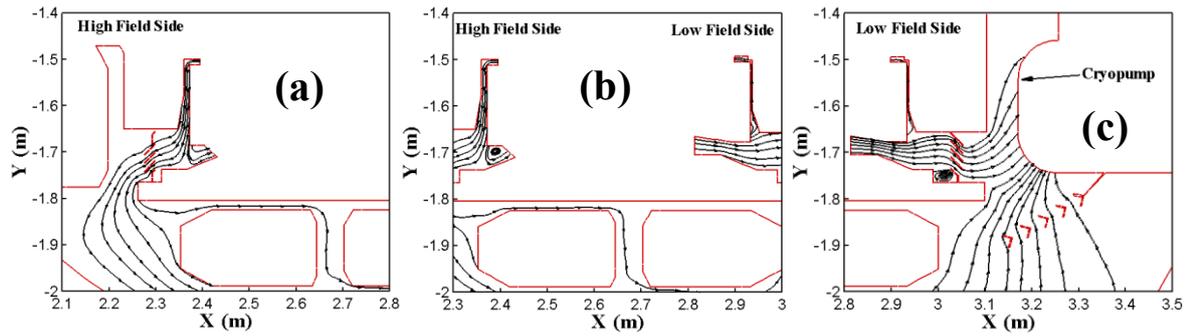


Figure 7: Streamlines of mixture (D and  $D_2$ ), for the case of (a) low, (b) medium and (c) high density cases.

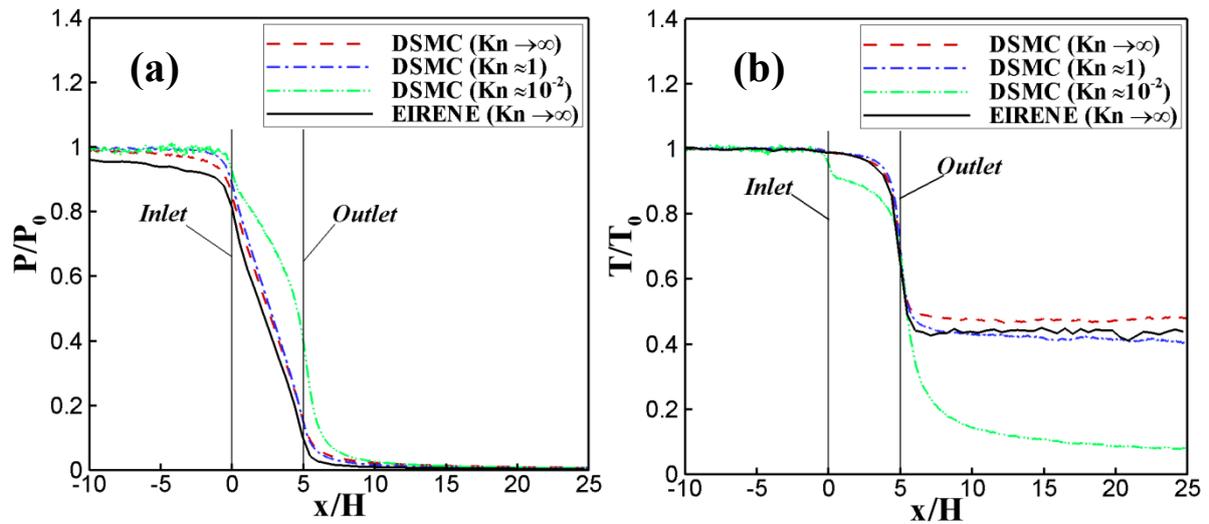
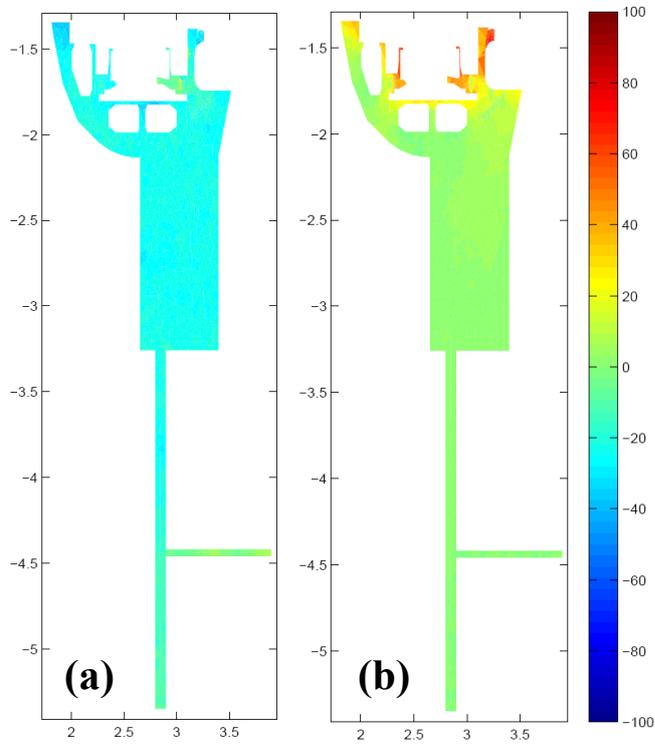


Figure 8: Comparison between DSMC [12] and EIRENE (a) dimensionless pressure and (b) temperature profiles along the symmetry axis  $y=0$ ; The presented configuration describes molecular deuterium gas flow through parallel plates with length to height ratio  $L/H=5$  and expansion into vacuum  $P_1/P_0=0$ . Three different

Knudsen numbers are chosen for comparison purposes, namely  $Kn \rightarrow \infty$ , 1 and  $10^{-2}$ , which cover the free molecular, transition and viscous flow regimes respectively. It is noted that  $P_0$ ,  $T_0$  is the reference pressure and temperature of the gas respectively, far away from the inlet of the parallel plates.



**Figure 9:** Relative percentage difference, defined as  $(X_{EIRENE} - X_{DIVGAS})/X_{DIVGAS}$ , between DIVGAS and collisionless EIRENE (a) number density and (b) temperature for molecular deuterium. The flow configuration corresponds to the highest value of the upstream density, equal to  $n_{e,sep,LFS-mp} = 1.1 \times 10^{19} (\text{m}^{-3})$ .