EFDA–JET–CP(14)06/37

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S. Varoutis[1], C. Gleason-González[1], D. Moulton[2], U. Kruezi[3], M. Groth[2], Chr. Day[1], S. Wiesen[4], D. Harting[3,4] and JET EFDA contributors*

JET-EFDA, Culham Science Centre, OX14 3DB, Abingdon, UK

[1]Karlsruhe Institute of Technology (KIT), Association EURATOM-KIT, Karlsruhe, Germany
[2]Aalto University, Association EURATOM-Tekes, Espoo, Finland
[3]EURATOM-CCFE Fusion Association, Culham Science Centre, OX14 3DB, Abingdon, OXON, UK
[4]IEK4-Plasma Physics, Forschungszentrum Jülich, Jülich ,Germany
** See annex of F. Romanelli et al, "Overview of JET Results",*
(25th IAEA Fusion Energy Conference, St Petersburg, Russia (2014)).

Preprint of Paper to be submitted for publication in Proceedings of the
25th IAEA Fusion Energy Conference, St Petersburg, Russia
13th October 2014 - 18th October 2014

ABSTRACT.
The present work includes 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 the KT5P pressure gauge. The Direct Simulation Monte Carlo (DSMC) code is able to predict qualitatively and quantitatively 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 strongly non-isothermal and covers the free molecular up to the transition flow regime. The relative difference between the measured pressure and the pressure in the sub-divertor area varies between 6-40% depending on the gas species and the plasma upstream conditions. Furthermore, for low and medium electron upstream density simulations, recirculation effects occur through gaps between the target tiles in the lower-high-field-side while for the highest electron upstream density case recirculation occurs only through gaps in the upper-low-field-side.

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. 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 and more important especially in cases where the plasma is almost always heavily influenced by plasma-wall interactions (the recycling flux usually dominates over 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 impurity neutrals into the core etc.). Depending on the plasma conditions, the neutral gas flow starts from continuum and slip regimes above the dome and close to the divertor targets and then covers transitional regime and even free molecular (collisionless) regime in the sub-divertor area. 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, the code package which is often used in the JET activities on fluid edge plasma modeling is the EDGE2D-EIRENE code [1], where the EDGE2D part consists of a 2D plasma fluid code, while the EIRENE algorithm [2] consists of a 3D Monte-Carlo solver for neutral-neutral interactions, based on the BGK kinetic model [3,4]. 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 for pressure driven isothermal flows. To describe more efficiently the non-isothermal flows (as the ones found in the sub-divertor region), we suggest in the present work the use of the Direct Simulation Monte Carlo method (DSMC) [5]. The DSMC approach is based on a particle method, in which the solution of the Boltzmann kinetic equation is circumvented 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 [6,7] 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. Just recently, a similar investigation on the ITER sub-divertor was performed by successfully implementing DSMC using SOLPS input data [8]. There, it was observed that high recirculation rates of neutrals behind the divertor targets occur. In view of DEMO, a reliable tool, which can predict the neutral recirculation and improve the exhaust pumping efficiency, is of vital importance. 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 DSMC algorithm. For validation purposes, the numerical values will be compared with existing JET ITER-Like Wall (ILW) [9] experimental data for the neutral gas pressure distribution in the sub-divertor region presented in [10]. The sub-divertor pressure measurements were obtained with a gauge located at the end of the main vertical lower port of Octant 8 (KT5P) [11]. The comparison between experiments and numerical data will be focused on three different L-mode plasma scenarios, which represent low, medium and high neutral gas divertor densities, respectively. For each case, the corresponding EDGE2D-EIRENE plasma simulations will be performed. Then, the information about the neutral particles on the interfaces along the divertor geometry will be extracted and imposed as boundary conditions (BC) for DSMC simulations. Following the above steps, the whole range of the Knudsen (Kn) number will be covered and it would be possible to quantify the differences between the numerical and experimental results in each regime.

2. DIVERTOR FLOW CONFIGURATION

The scope of this work is to examine the 2D behavior of the molecular and atomic deuterium binary gas mixture flow inside the JET sub-divertor domain. Figure 1 illustrates the performed 2D-cut of the 3D JET CATIA model of Octant No. 8. The cyan highlighted area in Fig.1 was chosen as the simulation domain for the DSMC calculations. Although the selected geometry is simplified, it still preserves the 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 end up to the pressure gauge position (KT5P). 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 300K, while the temperature of the vacuum vessel is assumed to be 473K. 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 before entering the sub-divertor area (i.e gas at rest with zero bulk velocity) and 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 (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 DSMC calculations an ideal pump was introduced where each particle that hits the surface of the pump is immediately absorbed. This corresponds to the limit case, in which the pump never saturates at maximum possible pumping speed.

3. EXPERIMENTAL SETTING

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. The JET ITER-like wall (JET-ILW) consists of Be-coated inconel tiles [9], including bulk Be in high heat flux areas, such as limiters, and Be-coated carbon-fibre 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 [10]. Furthermore, during the plasma discharge JET Pulse No: 81472 and as the upstream line-averaged density at the edge of the core plasma increases, the neutral gas pressure in the divertor is measured using the KT5P pressure gauge configuration. It is noted that in order to reduce the influence of the imposed magnetic field in the measurement resolution, the pressure devices are located far downwards from the sub-divertor structure (almost 2.5m away, see Fig. 2) and both locations communicate through a series of pipes and bellows. The KT5P configuration consists of two capacitance diaphragm gauges. The first device corresponds to a MKS 627D Baratron with pressure range of 0.1Torr and accuracy in reading of 0.12%, while the second device corresponds to a Pfeiffer CMR 365 with 0.1mbar pressure range and accuracy in reading of 0.5% [11]. 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 correspond only to MKS 627D Baratron measured data.

4. DSMC AND EDGE2D-EIRENE MODELLING

As has been shown in previous works [12-14], the DSMC method consists of a reliable and powerful tool for modelling rarefied gas flows. 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 modeled, i.e. their new coordinates $\boldsymbol{r}_{i,new}$ are estimated via the old ones $\boldsymbol{r}_{i,old}$ as.

  $\boldsymbol{r}_{i,new} = \boldsymbol{r}_{i,old} + \boldsymbol{v}_i \, \Delta t$

  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.

- 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

  $$N_{coil} = {}^{1}\!/_{2}\, N_p \overline{N}_p\, F_N \sigma_T v_{r,max} \; \frac{\Delta_t}{V_C}$$

  where N_p is the number of particles in a cell at that moment, $\overline{N}_p$ 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, σ_T is the total cross-section of the particle, $v_{r,\,max}$ 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 $\frac{v_r}{v_{r,\,max}} > R_f$, where v_r is the relative velocity of this pair and 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]. In VHS model the total cross section is a function of the relative velocity between two collided particles and the viscosity is proportional to T^{ω}, where the parameter ω is called viscosity index and characterizes a given gas. In the present work since molecular and atomic deuterium gases were considered, the viscosity index was taken 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 , the bulk velocity **u** and the temperature T in a computational cell are estimated by the following expressions,

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

  respectively. The final values of these quantities are given by the average amount during all time intervals Δt.

In the above framework, an unstructured computational grid which consists of $5\text{x}10^4$ triangular cells was applied in the computational field (Fig.2). In all the present simulations an optimum value of $\Delta t = 0.1\mu s$ has been used, which takes into account the fundamental criterion of DSMC that Δt 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 [15], 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 with a Maxwellian distribution function based on the wall temperature. The DSMC code used in the present work has been implemented in OpenFOAM, an open-source C++ tool box for computational fluid dynamics [16]. This solver, which is called *dsmcFoam*, has been rigorously validated for a variety of benchmark cases [17] and it has been modified accordingly for the purpose of the present work. The present DSMC code is fully parallelized and for all the presented calculations the high-performance computer "BwUniCluster" of Karlsruhe Institute of Technology (KIT) was used, by occupying up to 128 cores for each case.

The EDGE2D-EIRENE modeling corresponds to three different cases of upstream line-averaged density at the edge of the core plasma $\langle n_e \rangle_{l,edge}$, achieved by deuterium gas fuelling from the top and divertor (private flux) regions. All the cases, which were simulated, correspond to low-triangularity configurations ($\delta \sim 0.2$) [10] and represent cases with low, high and detached divertor conditions. In addition, it is noted that these cases correspond to low, medium and high collisionality in the sub-divertor area, respectively.

5. RESULTS AND DISCUSSION

In this section, the results obtained from the DSMC calculations and their comparison with corresponding experimental results of the KT5P pressure gauge are presented for the three 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 and a comparison between the calculated DSMC and KTP5 pressure measurements is conducted.

5.1 NEUTRAL GAS DYNAMICS IN THE JET SUB-DIVERTOR

In Fig.3a, the comparison between the calculated DSMC and measured molecular deuterium pressures at KT5P location, as a function of the line-averaged density at the edge is presented. As described in [10], by increasing $\langle n_e \rangle_{l,edge}$, the pressure at KT5P location increases exponentially over two decades. A similar behavior of the molecular deuterium pressure is reproduced by the DSMC results at the same location. Especially, for the case of $\langle n_e \rangle_{l,edge} = 2.2 \times 10^{19} (m^{-3})$, a factor of 2 between the calculated and measured values has been estimated. Taking into account all the assumptions and simplifications described in Section 2, it is clearly demonstrated that the DSMC method is able to efficiently describe real flow conditions of neutral gases even in such complex geometries.

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.3b, 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. For completeness, it is noted that 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 . For the given geometry, the height of the lower-LFS interface is equal to . The choice of this dimension as characteristic length is mainly based on the fact that in all three 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 and it is clearly seen that the temperature in the sub-divertor area is almost independent of the plasma conditions. Moreover, the flow field is proven 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 line-averaged density is presented. It is clearly seen that for the case of low , the *Kn* number is quite 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 the increases, then the *Kn* number decreases almost two order of magnitudes until the transition regime 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 particles 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 is presented. Since pressure is inverse proportional to the , 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 KT5P location and the calculated one in the sub-divertor area (location #3), shown in relative terms versus the line- averaged density in Fig. 5b. Based on this plot, it is deduced that only for the case of low densities the measured values of molecular D_2 represent the real values in the sub-divertor area with relative deviation of 6%. In all other density cases and gases, the relative difference may lie between 10 to 40% (i.e the pressure in location #3 is always higher than in the KT5P location, for each gas species). Such a discrepancy is mainly introduced due to the overall conductance of the lower port duct and the pipes ending up to the KT5P 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 KT5P measurements, or in the re-evaluation of previous data. Finally, an important qualitative observation regarding the behavior 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 6a, the gas mixture bulk velocity vector fields for the case of low density is presented and it is found that only in the Lower-HFS gap gas mixture is going towards the plasma chamber (see the direction of red arrows). Similar behavior is observed for the case of the medium density case. On the other hand, for the high density case (Fig.6b) recirculation of gas mixture takes place only in the Upper-LFS gap behind the divertor vertical targets (see the direction of red arrows).

SUMMARY

The present work includes a comparative study of the neutral gas dynamics in the JET sub-divertor. A complex model of the sub-divertor geometry is applied and successful comparisons between corresponding numerical and experimental data have been performed. The experimental data represent the neutral gas pressure obtained by the KT5P pressure gauge for an L-mode plasma case. The DSMC code is able to efficiently predict qualitatively and quantitatively the behaviour of the flow domain including macroscopic quantities of practical interest as the pressure and temperature. The numerical pressure coincides very well with the corresponding experimental values, within the experimental uncertainties. For all presented plasma cases, the deduced flow pattern is strongly non-isothermal. The relative difference between the measured neutral pressure at KT5P and the pressure in the sub-divertor area varies between 6-40 % depending on the gas species and the upstream line-averaged electron density. Furthermore, for low and medium electron density simulations, recirculation effects occur through a gap between the target tiles in the lower high-field-side while for the highest electron density case recirculation occurs only through another gap in the upper low-field-side. Consequently, such an investigation can be further exploited in view of DEMO preparation for enriching the understanding of the interaction between sub-divertor neutrals and the plasma core.

ACKNOWLEDGEMENT

This work was supported by EURATOM and carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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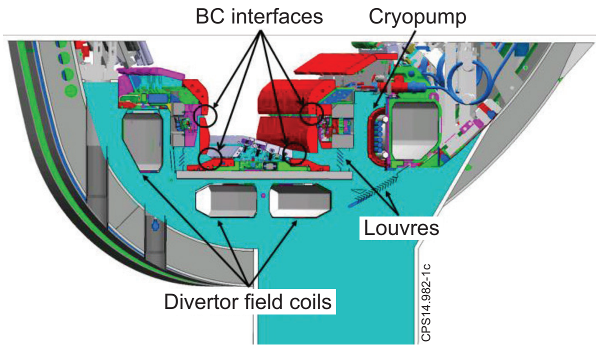


Figure 1: Geometrical representation of sub-divertor structure.

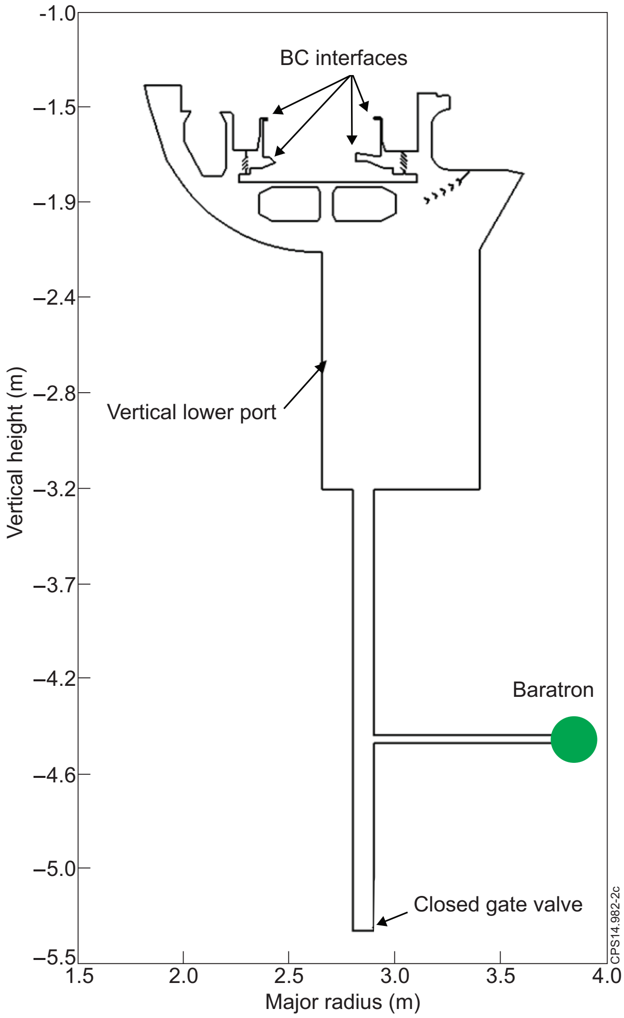
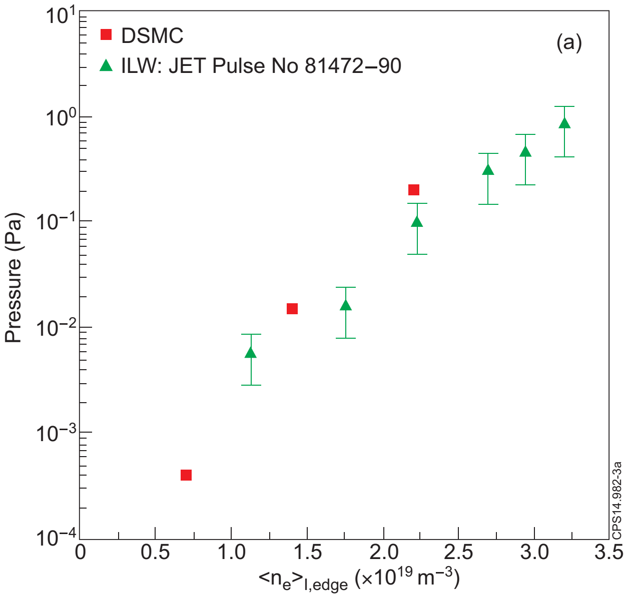


Figure 2: 2D model of the JET sub-divertor.



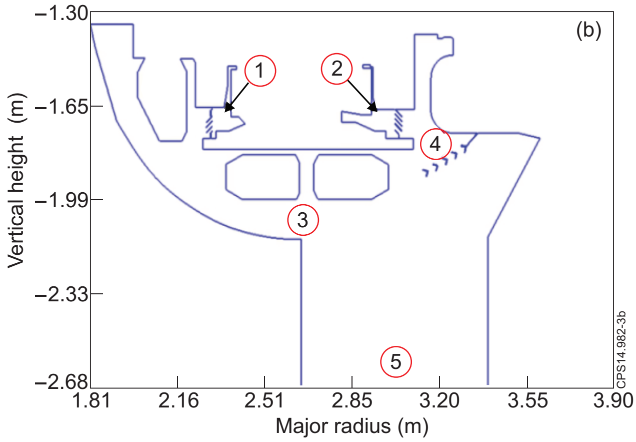
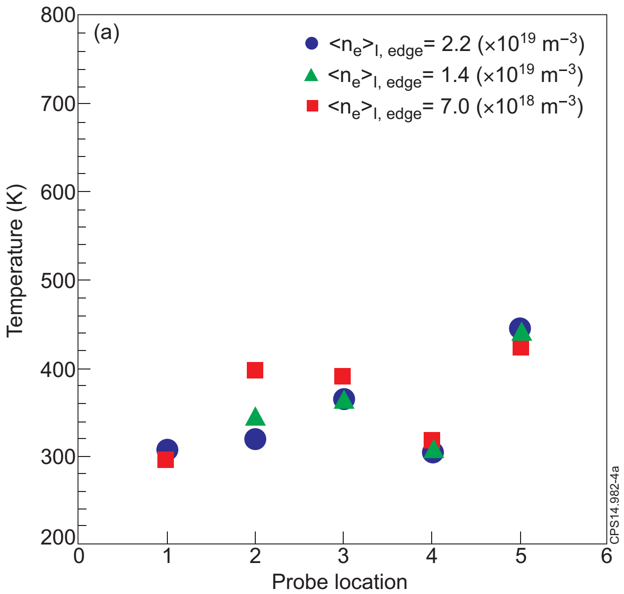


Figure 3: Comparison between the DSMC and experimental molecular deuterium pressure in the location of the KT5P gauge (a). Various locations (probes) in the sub-divertor area (b).



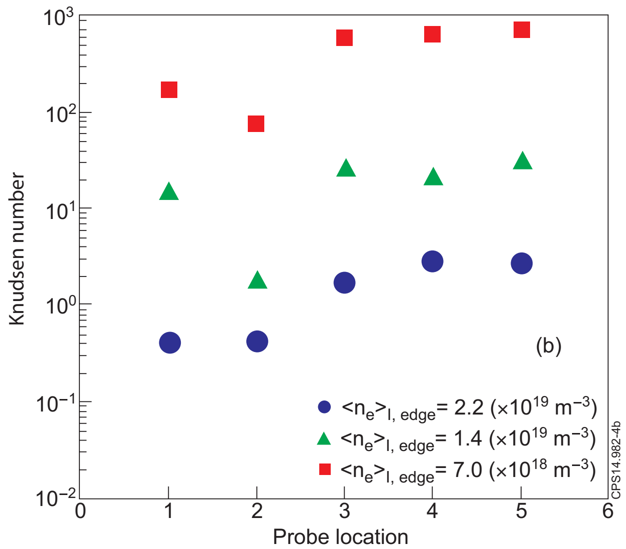


Figure 4: Overall temperature (a) and the local Kn number (b) for the gas mixture in various locations of the sub-divertor.

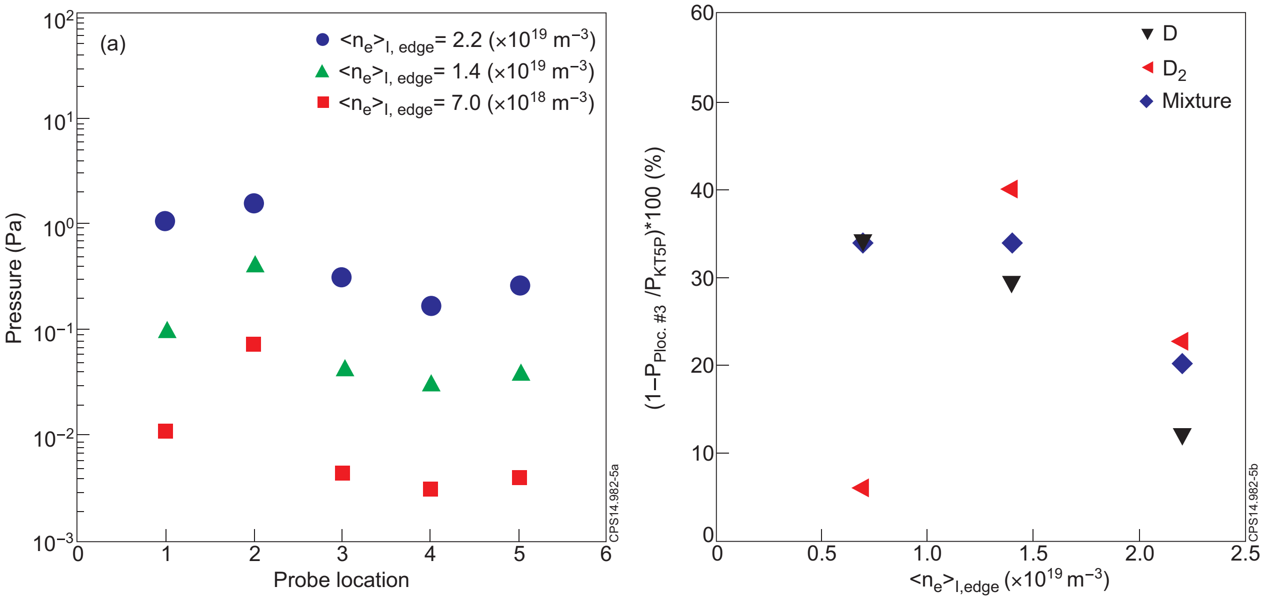


Figure 5: Pressure for gas mixture in various locations of the sub-divertor (a). Relative error between the KT5P pressure and the location #3 in the lower middle part of sub-divertor (b).

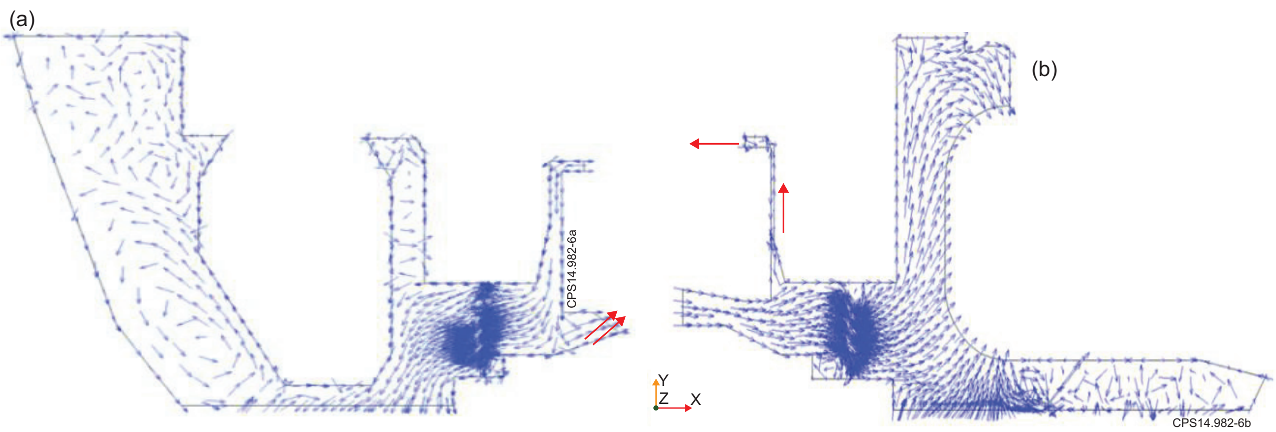


Figure 6: Gas mixture bulk velocity vector fields for low (a) and high (b) density cases.