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**Self-consistent simulation of turbulent transport
in the edge region of tokamaks
in diverted magnetic configuration**

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Abstract

The plasma dynamics in the region between the main plasma volume and the vessel wall has a strong influence on the overall performance of a tokamak fusion device. This region, called tokamak boundary, is characterized by high pressure gradients in a complex magnetic field geometry, resulting in nonlinear turbulent phenomena. In addition, the boundary is characterized by the presence of neutral particles, due to impurities in the volume, emitted by recycling at the wall or injected through puffing. The interaction between neutral particles and the plasma plays a key role in determining the dynamics of the tokamak boundary, providing sources and sinks of plasma particles and energy.

Leveraging the work in Corrado and Ricci [Nucl. Fusion **62**, 036015 (2022)], this thesis presents the first GBS simulations of a diverted plasma with a self-consistent model to simulate the interplay between neutrals and plasma in the tokamak boundary, carried out first with a single-ion species model, then with a multi-component one. The simulation are used to reconstruct phenomena observed in high-density L-mode tokamak discharges, in particular studying density shoulder formation and transport in detached conditions.

The GBS code allows for self-consistent three-dimensional numerical simulations of the turbulent plasma and neutral dynamics in the tokamak boundary. A set of Braginskii equations in the drift limit describes the plasma time evolution, and the neutrals are modelled by solving a kinetic equation using the method of characteristics. Recently, a multi-component model of the neutral-plasma interaction was developed by extending the single ion species one, allowing the description of a deuterium plasma that includes electrons, D^+ ions, D atoms, D_2^+ ions and D_2 molecules. The molecular dynamics in the plasma is introduced through a set of drift-reduced Braginskii equations for the D_2^+ species, coupled with the neutral particles modelling a set of processes that includes ionization, recombination, charge-exchange and dissociation processes.

By simulating a plasma composed by a single ion and single neutral species, the effect of increased core fuelling on the boundary density and temperature profile is investigated. The increase in core fuelling reproduces experimental measurements of higher plasma density in the far scrape-off layer (SOL) and increased e-folding length close to the separatrix. By an analysis of the particle balance in the SOL, the physical mechanisms underlying the increase of the far SOL density are analyzed, concluding that it is caused by the strong decrease of parallel transport. The effect of increased neutral density is to increase plasma cooling due to ionization events, leading ultimately to lower parallel velocities.

The multi-component model is applied to simulations of high-density deuterium plasmas in a lower single-null magnetic configuration based on a TCV discharge. To control the divertor conditions, a D_2 puffing is used and the effect of increased fuelling through the increase in puffing strength is investigated. The introduction of molecular interactions leads to a strong decrease in plasma temperature and to lower particle and heat fluxes, causing the detachment of the inner target. Most D neutrals are produced by molecular activated recombination, while plasma temperature is set by ionization energy losses for $T_e > 3$ eV and by dissociation and charge-exchange losses for lower T_e . The analysis of particle and transport balance in the divertor volume shows that the decrease of particle flux is caused by a decrease of

local neutrals ionization and parallel velocity, both caused by the lower plasma temperature. The presence of strong electric fields in high-density plasmas is also investigated, revealing the role of the $E \times B$ drift in the asymmetries of the divertor targets and on outer mid-plane turbulence. Simulation results are in agreement with experimental observations of increased density decay length, attributed to decrease of parallel transport, together with increased turbulence size and radial velocity.

Key words: plasma physics, tokamak boundary, diverted configuration, plasma turbulence, fluid simulations, drift-reduced Braginskii model, kinetic neutral dynamics, neutral-plasma interaction, molecular dynamics, density shoulder, high-density discharge, detachment

Sommario

La dinamica del plasma nella regione interposta tra il volume principale e la parete di un tokamak, influenza fortemente la performance del reattore a fusione. Questo volume, chiamato bordo o boundary, è tipicamente caratterizzato da grandi gradienti di pressione in una geometria magnetica complicata, la cui interazione genera fenomeni non lineari e turbolenti. In aggiunta, nel bordo vi è un'alta densità di particelle neutre, date da impurità del plasma, riciclaggio alla parete o iniettate tramite gas puffing. Le reazioni tra neutri e plasma giocano un ruolo fondamentale nella dinamica del bordo dei tokamak, determinando l'intensità delle sorgenti di particelle ed energia nel plasma.

Sfruttando il lavoro presentato in Corrado and Ricci [Nucl. Fusion **62**, 036015 (2022)], in questa tesi vengono presentate le prime simulazioni eseguite tramite GBS di un plasma nella configurazione divertore, al quale viene accoppiato un modello auto-consistente di interazione con particelle neutre. Il modello descrive prima un plasma composto da una singola specie di ione, successivamente vengono presentate simulazioni di un plasma composto da più specie. Nelle simulazioni vengono osservati fenomeni tipicamente presenti in scariche di tokamak ad alta densità, in modo L. I risultati vengono utilizzati per studiare la formazione della *density shoulder* e il *detachment*.

GBS è un codice che permette la simulazione numerica di un plasma tridimensionale nel bordo di un tokamak, ricostruendone la dinamica turbolenta e l'interazione con la dinamica di particelle neutre. Un set di equazioni di Braginskii nel limite di drift descrive l'evoluzione del plasma, mentre i neutri sono modellati risolvendo l'equazione cinetica della loro funzione di distribuzione tramite il metodo delle caratteristiche. Recentemente è stato formulato un modello multi-componente, estendendo il modello a singola specie, che permette la ricostruzione di un plasma di deuterio composto da elettroni, ioni D^+ , atomi D, ioni D_2^+ e molecole D_2 . La dinamica molecolare è introdotta tramite un set di equazioni di Braginskii nel limite di drift per la specie D_2^+ , accoppiata con le particelle neutre tramite reazioni di ionizzazione, ricombinazione, scambio di carica e dissociazione.

Tramite simulazioni di plasma composto da elettroni, ioni D^+ e atomi D, viene studiato l'effetto dell'aumento della sorgente di particelle nel core del tokamak, sulla densità e temperatura nel bordo. I risultati delle simulazioni riproducono qualitativamente le misure osservate sperimentalmente, come la densità aumentata nello scrape-off layer (SOL) e l'aumento della lunghezza di decadimento del profilo di pressione alla separatrice. Analizzando il bilancio di particelle nel SOL, i meccanismi fisici sottostanti l'aumento di densità vengono analizzati, concludendo che la sua causa primaria è la diminuzione del trasporto parallelo dal mid-plane al target. L'effetto dell'aumento della densità dei neutri è l'aumento della perdita di energia dovuto alla ionizzazione, portando alla diminuzione delle velocità parallele. Il modello multi-componente viene utilizzato per simulare un plasma di deuterio ad alta densità, in configurazione magnetica lower single-null, basata su una scarica del tokamak TCV. Le condizioni al divertore vengono controllate tramite un puffing di D_2 , usato per aumentare le sorgenti di particelle nelle simulazioni. L'introduzione delle interazioni molecolari portano ad una forte diminuzione della temperatura del plasma e minori flussi di particelle e calore, portando in ultimo al detachment del target interno. La maggior parte dei neutri D sono prodotti da ricombinazione molecolare, mentre la temperatura del plasma è controllata dalle perdite per ionizzazione per $T_e > 3$ eV e da dissociazione e

scambio di carica per T_e minori. L'analisi del trasporto nel volume del divertore mostra che la diminuzione del flusso di particelle è causata da una diminuzione della ionizzazione locale e della velocità parallela degli ioni, entrambe causate dalla temperatura ridotta. Viene investigata anche la presenza di campi elettrici nel plasma ad alta densità, rivelando il ruolo del drift $E \times B$ nella caratterizzazione delle asimmetrie tra i due target e sulla turbolenza al mid-plane. Le simulazioni sono in accordo con le osservazioni sperimentali riguardo le misure della velocità e dimensioni delle strutture turbolente.

Key words: fisica del plasma, bordo dei tokamak, configurazione divertore, turbolenza nel plasma, simulazioni fluide, equazioni di Braginskii, interazioni plasma-neutri, dinamica molecolare, density shoulder, scarica ad alta densità, detachment

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1 Introduction

In recent years human population has observed a constant increase in energy consumption, see Fig. 1.1. This trend results from the combination of increased world population and higher use of energy by a single person. Moreover, even if humanity could reduce energy consumption in a fraction of the world, in the near future growing countries will likely need to have access to more energy to improve their life quality (life expectation, education level, etc), see Fig. 1.2.

The majority of the current energy mix comes from fossil fuels, an energy source known to be problematic because of its limited reserves and for the correlation with the strong increase in atmospheric CO₂, with catastrophic consequences for the world climate [3]. Several different sources of energy have been explored in the last decades, the main one being biomass, geothermal, hydroelectricity, photovoltaic, wind and nuclear fission. Most of them suffer from intrinsic problems, such as limited capacity, intermittent availability, potential dangers or long lived waste, making them not competitive with fossil fuels.

1.1 Thermonuclear fusion for energy production

Since the early 20th century physicists are exploring a mechanism to produce energy that emulates stars: nuclear fusion. In this reaction, the fusion of two light nuclei produces heavier elements with a mass smaller than the sum of the total reactants mass, releasing an amount of energy proportional to this mass difference. On Earth, the few interesting fusion reactions for energy production involve the use of deuterium, that can be easily extracted from water, and tritium, that can be bred by lithium. The most appealing reaction for power plants [4] is



where the net energy production is 17.6 MeV, released as kinetic energy of the α particle (3.5 MeV) and neutron (14.1 MeV). It's interesting to notice that the fast neutron released could also be used to breed tritium directly inside the power plant, using it to produce the reaction fuel. From Eq. (1.1), it is clear that the reaction producing energy in a fusion reactor does not emit CO₂, is not dependant by location or weather and could be safely interrupted in case of emergency.

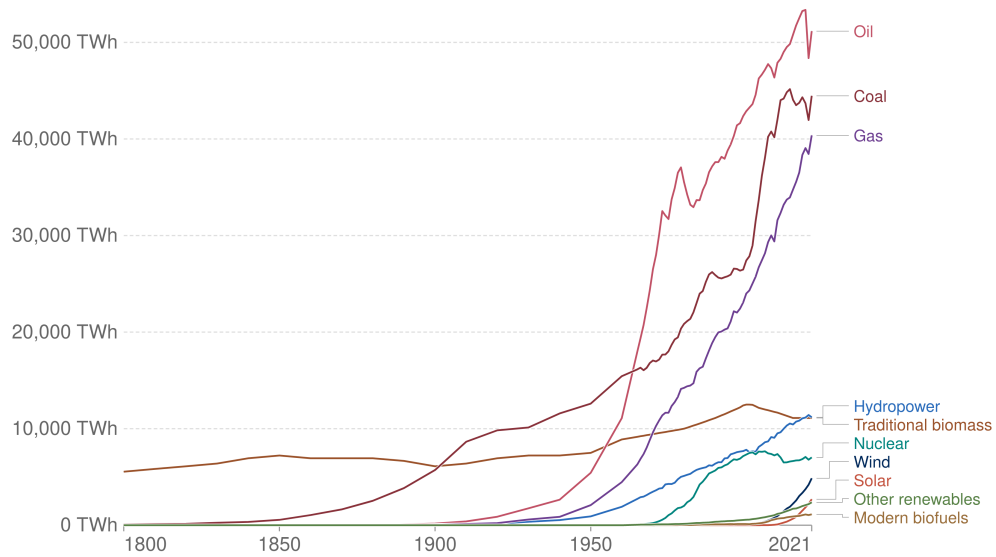


Figure 1.1: Global primary energy consumption by source, according to [1]. Image source: *ourworldindata.org*.

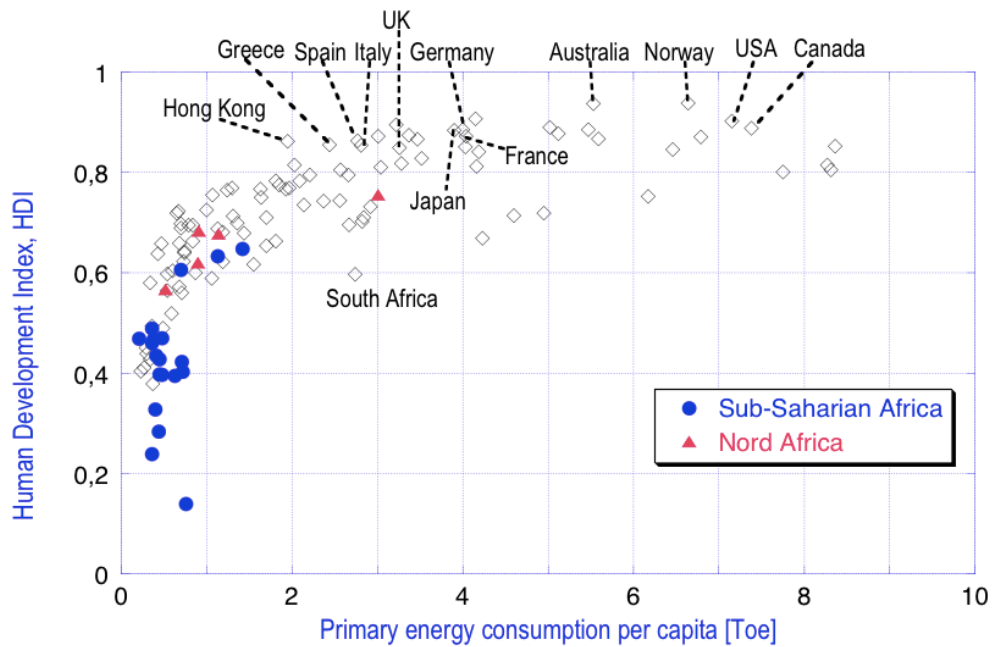


Figure 1.2: Human development index (HDI) vs energy consumption per capita. The HDI is a measure that combines life expectancy, education and GDP per capita [2].

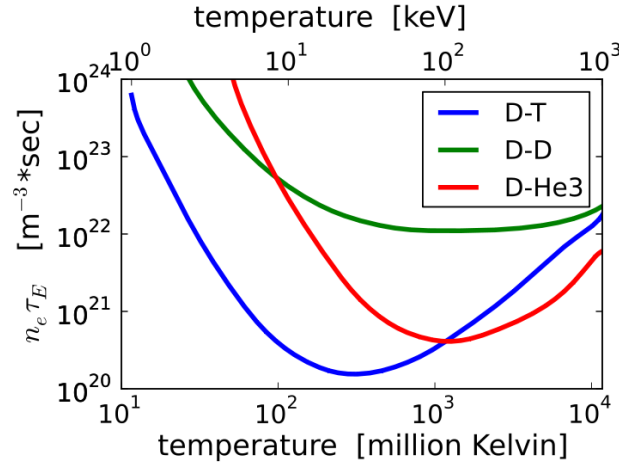


Figure 1.3: Product of plasma density and energy confinement time necessary to reach ignition. Source: [5]

For two nuclei to undergo a fusion reaction, they have to be in close proximity to each other, overcoming the Coulomb barrier that repels the protons. The only way to reduce the distance sufficiently is to have enough kinetic energy, i.e. for nuclear fusion to happen it is necessary to have extremely high temperatures, above million degrees. At those temperatures matter is in the state of *plasma*, where electrically charged particles live in a globally neutral medium gas. Inside this ionized gas, particles interact through long-range electromagnetic forces, producing collective behaviour. An estimate of the minimum plasma density and temperature necessary to produce enough fusion power to sustain the high temperatures, called *ignition*, can be found following Lawson's derivation [5]. The result is a relationship between plasma density n_e , ion temperature T_i and energy confinement time τ_E shown in Fig. 1.3, that can be summarized as

$$n_e T_i \tau_E \geq 5 \times 10^{21} \text{ s m}^{-3} \text{ keV}. \quad (1.2)$$

It's important to remark that the ignition condition is reached when the power lost from a fusion reactor is compensated by the power from the α -particles only, because they are the ones that contribute to heat the plasma. When the input power is compensated by the total produced energy, α plus neutrons, the condition is called *break-even*.

To satisfy the inequality in (1.2) one approach is to operate with high density plasma $n_e \simeq 10^{30} \text{ m}^{-3}$, for short times $\tau_E \simeq 10^{-10} \text{ s}$. This conditions are recreated in inertial confinement experiments, where high-power lasers hit high density pellets of deuterium and tritium, compressing it to produce a strong temperature and density increase. Recent progresses in the National Ignition Facility [6] showed promising results, producing more fusion energy (3.15 MJ) than the power injected by lasers (2.05 MJ). Another way to satisfy Lawson's criterion is to keep the plasma confined for long times $\tau_E \simeq 1 \text{ s}$, operating at lower plasma densities $n_e \simeq 10^{20} \text{ m}^{-3}$. The main idea is to exploit the Lorentz force to control the motion of charged particles, generating a magnetic field that confines the plasma. Because the Lorentz force act perpendicularly to the magnetic field, confinement can be reached in toroidal configuration [7], where particle drifts are kept in check winding the magnetic field lines around toroidal surfaces [4]. Based on how the magnetic field is obtained, toroidal devices can be distinguished between stellarators and tokamaks. The first one utilizes a set of external coils carefully manufactured to produce a complex non-planar shape, like in Wendelstein 7-X [8] or in the Large Helical Device [9]. In tokamaks the magnetic field is produced by a set of external coil and driving current inside the plasma

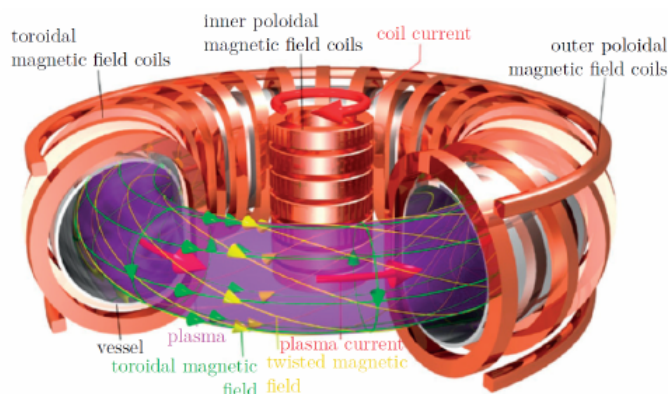


Figure 1.4: Schematic representation of a tokamak. Source: *EUROFusion website*.

by means of a central solenoid. Tokamaks are currently the most advanced devices for magnetic confinement fusion, with JET holding the record for highest fusion energy gain $Q = 0.67$ [10], defined as the ratio of fusion power over injected power. The most important future international fusion experiment is also a tokamak, ITER, which has the aim to demonstrate the feasibility of energy from fusion [11]. Despite the difficulties arising from the massive dimensions of the device and from the coordination of a cooperative work that includes all European Union, Japan, USA, China, Korea and India, ITER construction is currently undergoing in Cadarache, France. The goal of this experiment would be to reach $Q = 10$, producing 500 MW of power from an input of 50 MW [11].

1.2 The tokamak device

Fig. 1.4 shows a schematic representation of a tokamak. The toroidal magnetic field is generated by a set of planar toroidal coils, while the poloidal field is produced by driving current in the plasma. The current is produced by inducing a loop voltage in the plasma, thanks to the central solenoid. The twist introduced by the poloidal field is necessary to control particle drifts, that would arise with non-twisted circular lines, and improve particle confinement [4]. The plasma current running in the tokamak acts also as heating system for the plasma. This mechanism is however limited by the decrease of plasma resistivity at high temperature, limiting the allowed temperatures to few keV. Additional heating systems are necessary to reach higher temperatures [7].

Even if the single charged particles are confined by the magnetic field, collective behavior of the plasma due to Coulomb collision gives rise to transport across magnetic surfaces. In addition, transport in a tokamak is characterized by the complex interplay of several effects, like the existence of pressure gradients with curved magnetic field line, that trigger instabilities and leads to turbulence [12].

The typical description of a tokamak volume divides it in three regions denoted as core, edge and Scrape-Off Layer (SOL), as in Fig. 1.5. The first region is characterized by magnetic field lines wrapped around nested flux surfaces, closing on themselves. It is the hotter region of the volume, with the best confinement and where fusion reactions are expected to take place. The outer region of the volume is the SOL, characterized by magnetic field lines that intersect the tokamak vessel. The particle and heat fluxes going out from the core, due to the transport perpendicular to the

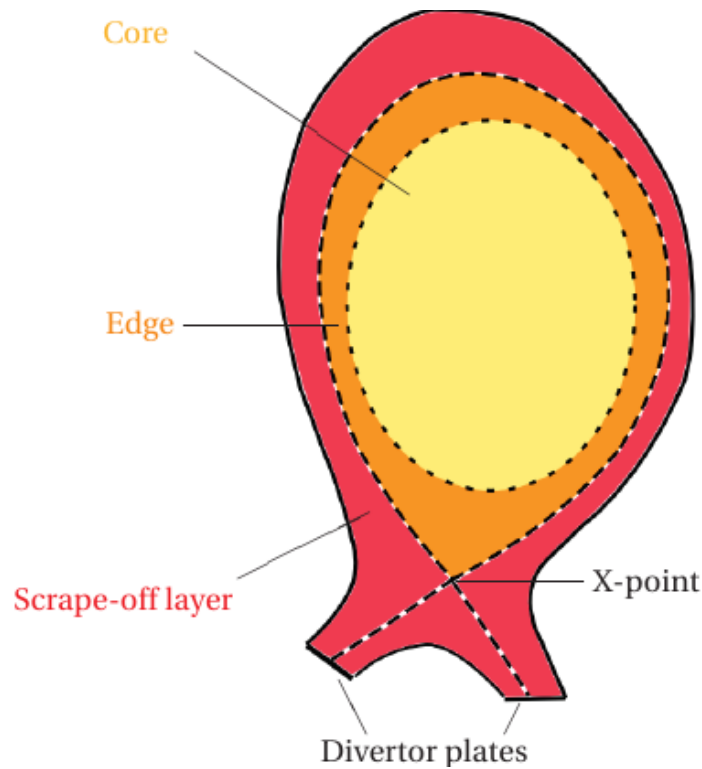


Figure 1.5: Poloidal section of a tokamak in diverted configuration. Source: [13].

magnetic flux surfaces, e.g. because of drifts or turbulence, enter the SOL and are deposited on the wall. The problem of avoiding damage to the vessel, especially around the plasma strike points, is often referred to as *power exhaust* problem and is still one of the main challenges that needs to be overcome for the construction of future power plants [14]. In order to control the position of the strike points, usually the magnetic field lines in the SOL are shaped by means of external coils, a configuration called *diverted* plasma. This configuration is characterized by the existence of one or more X-points where the poloidal magnetic field vanishes, an example is the Lower Single Null in Fig. 1.5. The last magnetic surface that intersects itself and sets the start of the SOL, is called Last Closed Flux Surface (LCFS). The goal of fusion power plant design is to have cold plasma (≈ 10 eV) in the SOL, while mounting complex divertor plates at the strike points, in order to withstand large heat fluxes. The region between the core and the SOL is the edge, characterized by closed magnetic field lines, but with steep pressure gradients, connecting the high pressure values in the core with the cold SOL. Those gradients are a source of energy for plasma instabilities, therefore the edge is characterized also by growing instabilities, with travelling eddies and turbulence. The possibility to have steeper gradients in the edge leads to the possibility to have higher core pressure, in other words plasma dynamics in the thin layer of the edge determines the overall performance of the tokamak.

1.3 Tokamak boundary and its modelling

The ensemble of edge and SOL is usually referred to as plasma boundary. The plasma physics in the boundary controls all the tokamak performance, sets the boundary condition for the core and controls heat exhaust, regulating plasma-wall

interaction.

The boundary is also characterized by the presence of neutrals interacting with the plasma. Neutrals are fundamental to control plasma fuelling and the level of impurities in the plasma [12], but they also introduce radiation losses useful for heat flux mitigation [15]. When plasma heats the walls, ions and electrons recombine and are recycled into the plasma as neutrals. A fraction of the ions can be simply reflected into the plasma, while another fraction can be absorbed and reemitted at a different temperature, depending on the material walls [16]. Neutrals going into the plasma are easily ionized in a hot and dense plasma, but neutral dynamics becomes more complex in the presence of cold plasma ≤ 3 eV. Moreover, the presence of different neutral and ion species quickly increases the possible interaction channels between plasma and neutrals, as represented in Fig. 1.6 for molecular deuterium.

The increase of plasma density usually leads to an increase of ionization close to the target plates, reducing the heat flux at the target. This regime, where heat transport is mainly conductive and the density source at the target balances the parallel particle flux, is often called high-recycling regime. A further increase of plasma density is usually followed by the increase of momentum losses and the activation of volumetric recombination, increasing neutral density while removing charged particles. The ultimate effect is the flattening of particle and heat fluxes at the target, in a regime called detachment, that is of particular interest for future tokamak operation [12].

The dynamics of the plasma boundary is strongly nonlinear, characterized by a range of time scales going from the gyro-motion ($\sim 10^{-9}$ s) to the energy confinement time (~ 1 s) and a range of lengths scales from the ion Larmor radius (~ 0.1 mm) to the machine size (~ 1 m). Moreover, the presence of turbulence means that the amplitude of the fluctuations have the same order of magnitude as equilibrium values, it is not possible to decouple average and fluctuating quantities. For those reasons, plasma transport modelling is extremely challenging.

In the SOL the low temperature makes the plasma collisional, where most often $k_{\parallel} \lambda_{\text{mfp}} \ll 1$, with $k_{\parallel}$ typical plasma perturbation wavenumber and λ_{mfp} electron mean free path. This allows a fluid description of the plasma dynamics, where a set of Braginskii equations can be used to evolve plasma density, velocity and temperature [17]. In the edge however the higher temperature breaks the collisional description, thus a fluid model will be valid only up to a certain position in the core. Simulations of plasma in the tokamak boundary are often based on fluid-diffusive models, that simplifies cross-field transport by means of a convective-diffusive approach, like in B2 [18, 19] or SOLEDGE-2D [20]. For neutrals it can be used a similar fluid approach, as in UEDGE [21], or a kinetic approach, usually based on Monte Carlo methods, as in DEGAS2 [22] or EIRENE [23]. The study and design of fusion devices as ITER strongly relies on simulations carried out by those codes and their coupling, like EMC3-EIRENE [24] and SOLPS-ITER [25].

In recent years, plasma turbulence simulations based on first-principles have emerged, overcoming the limitations of diffusive models. The codes running those simulations implement Braginskii equations, taken in the drift limit, like in BOUT++ [26], FELTOR [27], GRILLIX [28], SOLEDGE3X [29] and GBS [30, 31]. Some of the codes implement also a neutral model, simulating plasma-neutral interactions in the tokamak boundary, like in BOUT++ [32], in nHESEL [33, 34], in TOKAM3X-EIRENE [35] or in GBS [36, 37].

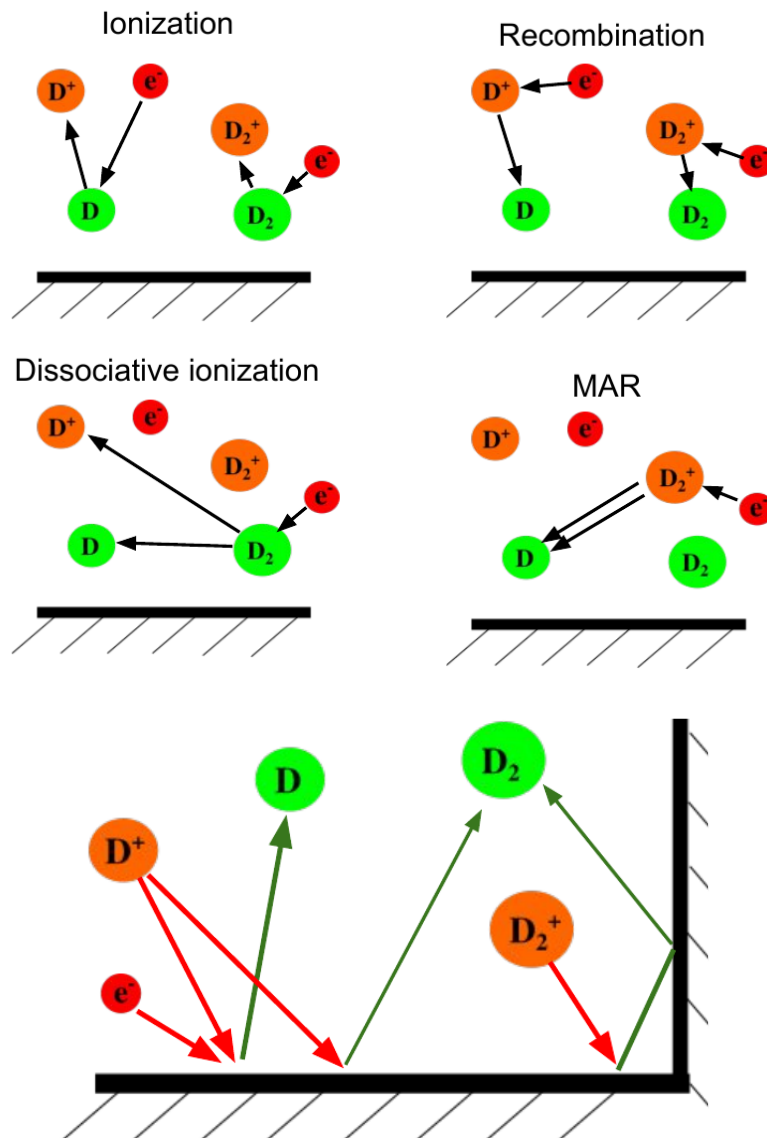


Figure 1.6: Representation of some of the possible reactions for a plasma composed by electrons and atomic and molecular deuterium ions, including molecular dissociation, Molecular Activated Recombination (MAR) and recombination at the wall (bottom). More details are explained in chapter 2.

1.4 Scope and outline of the thesis

The main goal of the present thesis is to investigate the effect of neutral-plasma interactions on the tokamak boundary equilibrium profiles and on turbulence, as they result from self-consistent plasma fluid simulations. The simulations are run with the Global Braginskii Solver (GBS), a three-dimensional global turbulence code that reconstructs plasma dynamics in a tokamak, based on the Braginskii equations [17] in the drift limit [38], without separation between fluctuations and equilibrium quantities. GBS is equipped with a neutral model that solves the kinetic Boltzmann equation for the neutral distribution functions, without recurring to Monte Carlo methods, thus avoiding statistical noise [36]. The present thesis addresses the problem of the description of plasma-neutral interactions in the SOL, implementing the neutral model in the version of the GBS code that simulates the full torus in an arbitrary magnetic configuration [31]. We remark that, up to now, the self-consistent neutral dynamics was resolved only in simulations with limited configuration [39, 37]. Moreover, the model is improved to be able to describe multiple ion fluids in diverted configuration, together with multiple neutral species. This model is then used in the thesis to shed light on the physics behind the phenomena observed in diverted experimental discharges with increasing fuelling. In particular, we reproduce the density shoulder formation and the transition toward the detachment regime, in different set of simulations. Plasma transport and turbulence are characterized, focusing on the interplay with neutral dynamics and the changes of parallel and perpendicular fluxes.

The present thesis is structured as follows. In Ch. 2, we present the last version of the GBS code [31], deriving the multi-species plasma model and solving the multi-species neutral model. We remark that the GBS code is now able to simulate electromagnetic effects, without using the Boussinesq approximation, in a diverted geometry and with the introduction of multiple ion and neutral species. In particular, the model is derived for atomic and molecular deuterium, since the molecular dynamics is expected to play an important role in plasma recycling and in detachment [40].

The first GBS simulation of self-consistent neutrals are shown in Ch. 3, where we reproduce plasma dynamics in a TCV-like LSN discharge to study the density shoulder formation. The flattening of the mid-plane pressure profile with increasing fuelling is reproduced by the simulations and analysed through particle balance, comparing parallel transport, perpendicular transport and local ionization sources. The increase in turbulent structure size with higher density is reproduced [41] and discussed through the comparison with simulations without neutral interactions. The experimental evidences in similar conditions are compared to our simulations results, together with theoretical scaling laws derived from other modelling studies.

In Ch. 4 we present the study of plasma transport in high-density simulations that includes molecular interactions. The plasma and neutral density profiles are discussed for different values of D_2 puffing and the main plasma energy sink mechanisms are analysed in details. The effect of increased neutral density on plasma transport in the divertor region is presented, showing the decrease of particle flux in the inner target of our configuration and the increased $E \times B$ transport. The plasma potential profile is set by the generalized Ohm's law, we analyze the effect of the density increase on the equation terms, in low plasma temperature conditions. The improvement of the algorithms used to detect turbulent structure allows us to determine with more accuracy their size and velocity, measuring an increase in both quantities for higher density.

Finally, the conclusions follows in chapter 5.

2 The GBS code for self-consistent plasma turbulence simulations

The present chapter describes the latest version of the GBS code. The plasma model allows the treatment of multiple ion species in a diverted configuration, on a domain that encompasses the whole tokamak volume, retaining the core-edge-SOL interplay. The neutral model solves the kinetic advection equations for multiple species, allowing self-consistent simulation of processes such as plasma recycling or gas puffing. The models describing the plasma and neutral species are coupled through a set of collisional interactions, which include ionization, charge-exchange, recombination and dissociation processes. In this chapter, the derivation of the two models is described for a plasma composed by three species, electrons, atomic deuterium ions, molecular deuterium ions, coupled with atomic and molecular deuterium. The case of single ion and neutral species is a reduction of the model and will be discussed at the end of this chapter. The implementation of the GBS multi-species model for a tokamak in diverted configuration is here presented in details for the first time, while the first simulation results are described in Ch. 4.

2.1 Introduction

The boundary of tokamak devices is characterized by the presence of multiple ion and neutral species, interacting through several collisional reactions [12]. Ions and electrons flow along the magnetic-field lines or across them, end at the vessel wall and recombine, re-entering the plasma volume as neutrals. A fraction of the resulting neutrals will keep the same energy as the impacting ion, they are *reflected*, while another fraction will be the result of wall absorption and are *reemitted* at wall temperature. Another possibility for impacting ions is to be absorbed by the wall, to associate and be emitted as a neutral molecule. The probability of undergoing one of these processes is determined by wall properties, e.g. in a metallic wall the reflected fraction is higher than in a Carbon wall [42, 40]. Neutral molecules can also be injected directly in the tokamak to fuel the plasma, to reduce heat flux at the targets [15] or for diagnostic purposes [43].

Once neutral atoms and molecules are in the tokamak volume, they will be ionized, producing atomic and molecular ions in a multi-component plasma. In this system, all the species can participate in several collision processes, like ionization, recombination, elastic collisions, charge-exchange and molecules dissociation, producing or destroying ion and neutrals. The complex interplay of these reactions plays a fundamental role in the multi-component plasma

turbulent dynamics. Simulations of tokamak boundary should properly take into account the multi-component nature of the plasma to accurately reconstruct and understand experimental observations.

A multi-component tokamak plasma is usually described by a fluid-diffusive model that consider a version of the Braginskii fluid equations simplified by modelling cross-field transport through empirical anomalous transport coefficients. This approach is used by several codes, like B2 [18, 19], EMC3 [24] or SOLEDGE-2D [20]. A similar fluid diffusive approach can be utilized for the neutral dynamics, when the neutral mean free path $\lambda_{\text{mfp},n}$ can be considered small. This approach is followed by codes like nHESEL, used for example to run single-ion simulation interacting with three neutral species [34, 33]. The limitation of the fluid approach are overcome using a kinetic description, usually relying on Monte Carlo methods. Those methods are used by several codes in different studies, like SOLPS-ITER to model a TCV density ramp [25] and the ASDEX detachment regimes [44] or with EDGE2D-EIRENE to model deuterium molecular emissions in DIII-D ohmic discharges [45]. Different models improve the description of perpendicular transport by using fluid and gyrofluid models to reproduce plasma turbulence, implemented for example in BOUT++ [26], FELTOR [27] or GRILLIX [28]. Simulations with multi-component turbulent plasma were carried out only in recent years, for example in the analysis of carbon impurities dynamics made with SOLEDGE3X (combination of SOLEDGE2D and TOKAM3X) [29] or the simulations of a gas puff imaging diagnostics in a limited tokamak with GBS [46].

In this chapter it is described the development and implementation in GBS of a multi-component model that addresses the plasma dynamics by means of a set of fluid drift-reduced Braginskii equations while describing the neutrals by a solving a kinetic advection equation for each species. GBS was initially developed to analyse plasma turbulence in basic plasma devices [47, 48], mainly studying simple magnetic devices like TORPEX [49] or LAPD [50]. During the years the model was improved, relaxing the cold ions and Boussinesq approximations [51], adding electromagnetic effects [52] and the coupling with a kinetic neutral model [36]. Finally, the present version of GBS uses a non-field-aligned coordinate system [53] that encompasses the whole tokamak volume, retaining all the core-edge-SOL interplay [31]. GBS can now also perform simulations of three dimensional magnetic equilibrium configurations such as the stellarator [54]. The use of a fluid model to describe the tokamak core lacks some fundamental elements, like kinetic effects, nonetheless it avoids unphysical phenomena appearing with the use of an artificial boundary [53] and improves the neutral interaction description, allowing the evaluation of the ionization inside the core [31]. The domain on the poloidal plane is a rectangular box, giving the possibility to simulate any kind of magnetic configuration, also retrieved from experimental discharges.

This work will present the first implementation of the GBS multi-species description with kinetic neutrals in a diverted configuration, exploiting the improvement of the latest version of the code [31] to extend the first results obtained by the multi-species model [37], to a diverted configuration. While the methodology to derive the model can be used for an arbitrary number of species, here it will be exploited to describe a deuterium plasma, composed by five species: electrons, e^- , atomic deuterium ions, D^+ , molecular deuterium ions, D_2^+ , atomic deuterium neutrals D and molecular deuterium neutrals D_2 . This model aims to simulate the basic processes happening in high density tokamak discharges, other species that could play additional roles in phenomena like detachment, e.g. D^- , will be neglected [40]. The kinetic neutral advection equations are solved by using the method of characteristics and integrating the formal solutions in velocity space. The system of coupled integral equations for neutral densities is then discretized, enabling its resolution and the possibility to retrieve all the higher-order moments of the kinetic equations. Taking advantage of the model implementation presented here, we will show the first simulations of a GBS high-density turbulent simulation in a lower single null TCV-like magnetic configuration in Ch. 4.

The chapter is organized as follows. The derivation of the fluid plasma model is first introduced in Sec. 2.2, summarizing the Braginskii model derivation and the use of Zdhanov closure for multiple ion species [55]. The coupling between plasma and neutral model is discussed in a dedicated subsection, where the terms arising from neutral interactions are described. The derivation of the plasma model concludes with the description of boundary conditions and its implementation inside the GBS code. Sec. 2.3 presents the kinetic neutral model, along with its resolution and implementation inside GBS. At the end, in Sec. 2.4, the chapter presents a discussion of the single ion and neutral species model, used in Ch. 3 of this thesis.

2.2 The plasma model

This section summarizes the derivation of the plasma model implemented in the GBS code. We start from the Braginskii equations, with the use of the drift approximation and the Zdhanov closure, then we will describe the plasma-neutral collisions considered and we will end with the complete set of equations.

2.2.1 Three-fluid Braginskii equations

All three species for the plasma are modelled by using a set of equations based on the Braginskii derivation [56]. Plasma dynamics is described using the kinetic Boltzmann equation for the distribution function of each species, including the terms arising from plasma-neutral interactions, yielding equations for f_e , f_{D^+} and $f_{D_2^+}$

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \frac{\partial f_i}{\partial \mathbf{x}} + q_i \left(\frac{\mathbf{E} + \mathbf{v} \times \mathbf{B}}{m_i} \right) \cdot \frac{\partial f_i}{\partial \mathbf{v}} = C_c(f_i) + C_n(f_i), \quad (2.1)$$

where $i = e, D^+ \text{ or } D_2^+$, q_i and m_i are the charge and the mass of the considered species, $\partial/\partial \mathbf{x}$ and $\partial/\partial \mathbf{v}$ denote the gradient in real and in velocity space, C_c denotes Coulomb collisions between charged species and C_n denotes collisions with neutral species.

The three-fluid Braginskii equations are obtained computing the first three moments of the kinetic equations, considering that the ion cyclotron motion is fast compared to the timescale of Coulomb collision, i.e. $\Omega_{eD^+} \tau_{D^+} \gg 1$ with $\Omega_{eD^+} = eB/m_{D^+}$ ion cyclotron frequency. Density, average fluid velocity and temperature for each species are defined as

$$n_i = \int f_i d\mathbf{v}, \quad (2.2)$$

$$\mathbf{v}_i = \frac{1}{n_i} \int \mathbf{v} f_i d\mathbf{v} = \langle \mathbf{v} \rangle_i, \quad (2.3)$$

$$T_i = \frac{1}{n_i} \int \frac{m_i}{3} (\mathbf{v} - \mathbf{v}_i)^2 f_i d\mathbf{v} = \frac{m_i}{3} \langle (\mathbf{v} - \mathbf{v}_i)^2 \rangle_i, \quad (2.4)$$

leading to the Braginskii equations as presented in [57]:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{v}_e) = s_{n_e}, \quad (2.5)$$

$$\frac{\partial n_{D^+}}{\partial t} + \nabla \cdot (n_{D^+} \mathbf{v}_{D^+}) = s_{n_{D^+}}, \quad (2.6)$$

$$\frac{\partial n_{D_2^+}}{\partial t} + \nabla \cdot (n_{D_2^+} \mathbf{v}_{D_2^+}) = s_{n_{D_2^+}}, \quad (2.7)$$

$$m_e n_e \frac{d_e v_{e\alpha}}{dt} = -\frac{\partial p_e}{\partial x_\alpha} - \frac{\partial \Pi_{e\alpha\beta}}{\partial x_\beta} - en_e [E_\alpha + (\mathbf{v}_e \times \mathbf{B})_\alpha] + R_{e\alpha} + s_{v_{e\alpha}}, \quad (2.8)$$

$$m_D n_{D^+} \frac{d_{D^+} v_{D^+\alpha}}{dt} = -\frac{\partial p_{D^+}}{\partial x_\alpha} - \frac{\partial \Pi_{D^+\alpha\beta}}{\partial x_\beta} + en_{D^+} [E_\alpha + (\mathbf{v}_{D^+} \times \mathbf{B})_\alpha] + R_{D^+\alpha} + s_{v_{D^+\alpha}}, \quad (2.9)$$

$$m_{D_2} n_{D_2^+} \frac{d_{D_2^+} v_{D_2^+\alpha}}{dt} = -\frac{\partial p_{D_2^+}}{\partial x_\alpha} - \frac{\partial \Pi_{D_2^+\alpha\beta}}{\partial x_\beta} + en_{D_2^+} [E_\alpha + (\mathbf{v}_{D_2^+} \times \mathbf{B})_\alpha] + R_{D_2^+\alpha} + s_{v_{e\alpha}}, \quad (2.10)$$

$$\frac{3}{2} n_e \frac{d_e T_e}{dt} + p_e \nabla \cdot \mathbf{v}_e = -\nabla \cdot \mathbf{q}_e - \Pi_{e\alpha\beta} \frac{\partial v_{e\beta}}{\partial x_\alpha} + Q_e + s_{T_e}, \quad (2.11)$$

$$\frac{3}{2} n_{D^+} \frac{d_{D^+} T_{D^+}}{dt} + p_{D^+} \nabla \cdot \mathbf{v}_{D^+} = -\nabla \cdot \mathbf{q}_{D^+} - \Pi_{D^+\alpha\beta} \frac{\partial v_{D^+\beta}}{\partial x_\alpha} + Q_{D^+} + s_{T_{D^+}}, \quad (2.12)$$

$$\frac{3}{2} n_{D_2^+} \frac{d_{D_2^+} T_{D_2^+}}{dt} + p_{D_2^+} \nabla \cdot \mathbf{v}_{D_2^+} = -\nabla \cdot \mathbf{q}_{D_2^+} - \Pi_{D_2^+\alpha\beta} \frac{\partial v_{D_2^+\beta}}{\partial x_\alpha} + Q_{D_2^+} + s_{T_{D_2^+}}, \quad (2.13)$$

where $\Pi_{e\alpha\beta}$ denotes the component of the stress tensor along the α and β directions, $\mathbf{R}_e$ the friction force acting on the electrons, $\mathbf{q}_e$ the electron heat flux density, Q_e the electron heat generated by Coulomb collisions and $d_e/dt = \partial/\partial t + (\mathbf{v}_e \cdot \nabla)$ the electron advective derivative. The equivalent notation is used for the D^+ and D_2^+ species. The source terms s_k for each quantity k are contributes given by neutral collisions and will be discussed in Sec. 2.2.2.

In the typical conditions of tokamak boundaries, it is possible to consider the ion cyclotron motion faster than the characteristic timescales we are interested in, i.e. $d/dt \ll \Omega_{cD^+}$. Moreover, the ion Larmor radius can be considered shorter than the characteristic turbulent perpendicular length, i.e. $k_\perp \rho_{sD^+} \ll 1$. These approximations lead to the drift-limit of the Braginskii equations, where only the leading components in $(1/\Omega_{cD^+})d/dt$ of the perpendicular velocities are kept. For the electron velocity it results $\mathbf{v}_{\perp e} = \mathbf{v}_{\perp e0} = \mathbf{v}_{E \times B} + \mathbf{v}_{de}$, with $E \times B$ drift $\mathbf{v}_{E \times B} = (\mathbf{E} \times \mathbf{B})/B^2$ and electron diamagnetic drift $\mathbf{v}_{de} = (\mathbf{B} \times \nabla p_e)/(en_e B^2)$, for the D^+ ions to $\mathbf{v}_{\perp D^+} = \mathbf{v}_{E \times B} + \mathbf{v}_{dD^+} + \mathbf{v}_{pol,D^+} + \mathbf{v}_{fric,D^+}$,

with $\mathbf{v}_{dD^+} = (\mathbf{B} \times \nabla p_{D^+}) / (en_{D^+} B^2)$. The polarization drift can be written as [38, 37]

$$\begin{aligned} \mathbf{v}_{\text{pol}, D^+} = & \frac{\mathbf{b}}{\Omega_{cD^+}} \times \frac{d}{dt} \mathbf{v}_{\perp D^+ 0} + \frac{1}{n_{D^+} m_{D^+} \Omega_{cD^+}} \left\{ \mathbf{b} \times \left[p_{D^+} \left(\nabla \times \frac{\mathbf{b}}{\Omega_{cD^+}} \right) \cdot \nabla v_{\perp D^+ 0} \right] \right. \\ & + \mathbf{b} \times \nabla_{\perp} \left(\frac{p_{D^+}}{2\Omega_{cD^+}} \nabla \cdot \mathbf{b} \times \mathbf{v}_{\perp D^+ 0} \right) - \nabla_{\perp} \left(\frac{p_{D^+}}{2\Omega_{cD^+}} \nabla_{\perp} \cdot \mathbf{v}_{\perp D^+ 0} \right) \Big\} \\ & + \frac{1}{n_{D^+} m_{D^+} \Omega_{cD^+}} \mathbf{b} \times \left(G_{D^+} \mathbf{k} - \frac{\nabla G_{D^+}}{3} \right), \end{aligned} \quad (2.14)$$

where in the time derivative the polarization and friction velocities are neglected due to the drift ordering, the magnetic field curvature is defined as $\mathbf{k} = (\mathbf{b} \cdot \nabla) \mathbf{b}$ and the gyroviscous term is

$$G_{D^+} = -\eta_{0D^+} \left(2\nabla_{\parallel} v_{\parallel D^+} + \frac{C(\phi)}{B} + \frac{C(p_{D^+})}{en_{D^+} B} \right), \quad (2.15)$$

with parallel gradient $\nabla_{\parallel} = \mathbf{b} \cdot \nabla$ and $\mathbf{b} = \mathbf{B}/B$. The same approach is utilised also for D_2^+ ions, with similar definitions.

To close the Braginskii equations, Eqs. (2.6-2.13), an expression for the parallel friction forces and the heat fluxes is obtained following the procedure developed by Zdhanov [58, 59]. It is assumed that friction forces and heat fluxes are proportional to parallel gradients of temperatures and parallel velocities:

$$\begin{pmatrix} q_{\parallel \alpha} \\ R_{\parallel \alpha} \end{pmatrix} = \sum_{\beta} Z_{\alpha\beta} \begin{pmatrix} \nabla_{\parallel} T_{\beta} \\ w_{\parallel \beta} \end{pmatrix}, \quad (2.16)$$

with α and β indexes of the plasma species and w_{β} the parallel component of the fluid velocity of species β with respect to the center of mass of the plasma $\mathbf{w}_{\beta} = \mathbf{v}_{\beta} - (\sum_{\gamma} n_{\gamma} m_{\gamma} \mathbf{v}_{\gamma}) / (\sum_{\gamma} n_{\gamma} m_{\gamma})$. The matrix $Z_{\alpha\beta}$ is then found under the assumptions of quasi-neutrality $n_e = n_{D^+} + n_{D_2^+}$, of $n_{D_2^+}/n_{D^+} \ll 1$, keeping only the leading order in $\sqrt{m_e/m_{D^+}}$ and $T_{D^+} \simeq T_e$. The final expressions are [37]

$$\begin{aligned} R_{\parallel e} &= -0.71 n_e \nabla_{\parallel} T_e - \frac{0.51 m_e n_e}{\tau_{eD}} (v_{\parallel e} - v_{\parallel D^+}), \\ R_{\parallel D^+} &= 0.71 n_e \nabla_{\parallel} T_e - \frac{0.51 m_e n_e}{\tau_{eD}} (v_{\parallel D^+} - v_{\parallel e}), \\ R_{\parallel D_2^+} &= 0, \\ q_{\parallel e} &= -\frac{3.16 n_e T_e \tau_{eD}}{m_e} \nabla_{\parallel} T_e + 0.71 n_e T_e (v_{\parallel e} - v_{\parallel D^+}), \\ q_{\parallel D^+} &= -\frac{4.52 n_e T_{D^+} \tau_{eD}}{\sqrt{2 m_e m_{D^+}}} \nabla_{\parallel} T_{D^+}, \\ q_{\parallel D_2^+} &= -\frac{1.80 n_e T_{D^+} \tau_{eD}}{\sqrt{2 m_e m_{D^+}}} \nabla_{\parallel} T_{D^+}, \end{aligned} \quad (2.17)$$

where τ_{eD^+} is the characteristic time scale of collisions between electrons and D^+ ions.

Under the above given assumptions the continuity equation for the density of electrons and D_2^+ becomes

$$\frac{\partial n_e}{\partial t} + \nabla \cdot [n_e (\mathbf{v}_{E \times B} + \mathbf{v}_{de} + v_{\parallel e} \mathbf{b})] = s_{n_e}, \quad (2.18)$$

$$\frac{\partial n_{D_2^+}}{\partial t} + \nabla \cdot [n_{D_2^+}(\mathbf{v}_{E \times B} + \mathbf{v}_{dD_2^+} + \mathbf{v}_{pol} + v_{\parallel D_2^+} \mathbf{b} + \mathbf{v}_{fricD_2^+})] = s_{n_{D_2^+}}, \quad (2.19)$$

while the D^+ ion density is found imposing quasi-neutrality $n_{D^+} = n_e - n_{D_2^+}$.

The assumption of quasi-neutrality can be used to find also the vorticity equation

$$\begin{aligned} \nabla \cdot (n_{D^+} \mathbf{v}_{D^+} + n_{D_2^+} \mathbf{v}_{D_2^+}) + \frac{1}{e} \nabla_{\parallel} j_{\parallel} + \nabla \cdot [n_{D^+} \mathbf{v}_{dD^+} + n_{D_2^+} \mathbf{v}_{dD_2^+} - n_e \mathbf{v}_{de}] \\ + \nabla \cdot (n_{D^+} \mathbf{v}_{fric,D^+} + n_{D_2^+} \mathbf{v}_{fric,D_2^+}) = 0, \end{aligned} \quad (2.20)$$

that is equivalent to $\nabla \cdot \mathbf{j} = 0$. Writing the expression for the polarization drifts, Eq. (2.14), leads to the equation for the evolution of the electric field $\mathbf{E}_{\perp}$.

Electromagnetic effects are taken into account under the assumption of small-amplitude magnetic perturbations and observing that the typical turbulence scale length in the parallel direction is much longer than the one in the perpendicular direction. The resulting Ampère equation is

$$\nabla_{\perp}^2 \psi = \mu_0(j_{\parallel} - \bar{j}_{\parallel}), \quad (2.21)$$

where we define $\psi = -\delta A_{\parallel}$, perturbation of the parallel component of the potential vector and $\bar{j}_{\parallel}$ the average electric current.

The parallel momentum equation for electrons and ions is evaluated projecting Eqs. (2.8-2.10) along the parallel direction, while the temperature equations are derived from Eqs. (2.11-2.13) applying the drift-ordering and neglecting the viscous heat losses. The resulting set of equations is

$$\frac{\partial n_e}{\partial t} = -\frac{1}{B}[\phi, n_e] + \frac{2}{eB}[C(p_e) - en_e C(\phi)] - \nabla_{\parallel}(n_e v_{\parallel e}) + \mathcal{D}_{n_e} \nabla_{\perp}^2 n_e + s_{n_e}, \quad (2.22)$$

$$\begin{aligned} \frac{\partial n_{D_2^+}}{\partial t} = -\frac{1}{B}[\phi, n_{D_2^+}] - \nabla_{\parallel}(n_{D_2^+} v_{\parallel D_2^+}) - \frac{2}{eB}[C(p_{D_2^+}) + en_{D_2^+} C(\phi)] \\ + \mathcal{D}_{n_{D_2^+}} \nabla_{\perp}^2 n_{D_2^+} + s_{n_{D_2^+}}, \end{aligned} \quad (2.23)$$

$$\begin{aligned} \frac{\partial \Omega}{\partial t} = -\frac{1}{B} \nabla \cdot ([\phi, \omega_{D^+}] + 2[\phi, \omega_{D_2^+}]) - \nabla \cdot (v_{\parallel D^+} \nabla_{\parallel} \omega_{D^+} + v_{\parallel D_2^+} \nabla_{\parallel} \omega_{D_2^+}) \\ + \frac{2\Omega_{cD^+}}{e} C(p_e + p_{D^+} + p_{D_2^+}) + \frac{B\Omega_{cD^+}}{e} \nabla_{\parallel} j_{\parallel} + \frac{\Omega_{cD^+}}{3e} C(G_{D^+} + G_{D_2^+}) \\ + \eta_0 \nabla_{\parallel}^2 \Omega + \mathcal{D}_{\Omega} \nabla_{\perp}^2 \Omega + s_{\Omega}, \end{aligned} \quad (2.24)$$

$$\begin{aligned} \frac{\partial U_{\parallel e}}{\partial t} = -\frac{1}{B}[\phi, v_{\parallel e}] + \frac{e}{m_e} \left[\frac{j_{\parallel}}{\sigma_{\parallel}} + \nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_e}{en_e} - \frac{2}{3n_e} \nabla_{\parallel} G_e - \frac{0.71}{e} \nabla_{\parallel} T_e \right] \\ - v_{\parallel e} \nabla_{\parallel} v_{\parallel e} + \mathcal{D}_{v_{\parallel e}} \nabla_{\perp}^2 v_{\parallel e} + s_{v_{\parallel e}}, \end{aligned} \quad (2.25)$$

$$\begin{aligned} \frac{\partial v_{\parallel D^+}}{\partial t} = -\frac{1}{B}[\phi, v_{\parallel D^+}] - v_{\parallel D^+} \nabla_{\parallel} v_{\parallel D^+} - \frac{e}{m_{D^+}} \nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_{D^+}}{m_{D^+} n_{D^+}} \\ - \frac{2}{3n_{D^+}} \nabla_{\parallel} G_{D^+} + \frac{0.71}{m_{D^+} n_{D^+}} \nabla_{\parallel} T_e - \frac{en_e}{m_{D^+} n_{D^+}} \frac{j_{\parallel}}{\sigma_{\parallel}} + \mathcal{D}_{v_{\parallel D^+}} \nabla_{\perp}^2 v_{\parallel D^+} + s_{v_{\parallel D^+}}, \end{aligned} \quad (2.26)$$

$$\begin{aligned} \frac{\partial v_{\parallel D_2^+}}{\partial t} = & -\frac{1}{B}[\phi, v_{\parallel D_2^+}] - v_{\parallel D_2^+} \nabla_{\parallel} v_{\parallel D_2^+} + \frac{e}{2m_{D^+}} \left[-\nabla_{\parallel} \phi - \frac{\nabla p_{D_2^+}}{en_{D_2^+}} - \frac{2}{3en_{D_2^+}} \nabla_{\parallel} G_{D_2^+} \right] \\ & + \mathcal{D}_{v_{\parallel D_2^+}} \nabla_{\perp}^2 v_{\parallel D_2^+} + s_{v_{\parallel D_2^+}} \quad , \end{aligned} \quad (2.27)$$

$$\begin{aligned} \frac{\partial T_e}{\partial t} = & -\frac{1}{B}[\phi, T_e] - v_{\parallel e} \nabla_{\parallel} T_e + \frac{4T_e}{3eB} \left[\frac{7}{2} C(T_e) + \frac{T_e}{n_e} C(n_e) - eC(\phi) \right] - \frac{2T_e}{3} \nabla_{\parallel} v_{\parallel e} \\ & + \frac{2m_{D^+}}{3en_e} [1.62\sigma_{\parallel} \nabla_{\parallel} (n_e T_e \nabla_{\parallel} T_e) - 0.71 \nabla_{\parallel} (T_e j_{\parallel})] \\ & + \chi_{\perp e} \nabla_{\perp}^2 T_e + \nabla_{\parallel} (\chi_{\parallel e} \nabla_{\parallel} T_e) + s_{T_e} \quad , \end{aligned} \quad (2.28)$$

$$\begin{aligned} \frac{\partial T_{D^+}}{\partial t} = & -\frac{1}{B}[\phi, T_{D^+}] - v_{\parallel D^+} \nabla_{\parallel} T_{D^+} + \frac{4}{3} \frac{T_{D^+}}{eB} \left[\frac{1}{n_{D^+}} C(p_e + p_{D_2^+}) - eC(\phi) \right] \\ & - \frac{2T_{D^+}}{3n_{D^+}} \left[\nabla_{\parallel} (n_e v_{\parallel e}) - \nabla_{\parallel} (n_{D_2^+} v_{\parallel D_2^+}) - v_{\parallel D^+} \nabla_{\parallel} (n_{D_2^+}) \right] \\ & - \frac{10}{3} \frac{T_{D^+}}{eB} C(T_{D^+}) + \frac{2.32\sqrt{2m_e m_{D^+}}}{3} \frac{\sigma_{\parallel}}{en_{D^+}} \nabla_{\parallel} (n_e T_{D^+} \nabla_{\parallel} T_{D^+}) \\ & + \chi_{\perp D^+} \nabla_{\perp}^2 T_{D^+} + \nabla_{\parallel} (\chi_{\parallel D^+} \nabla_{\parallel} T_{D^+}) + s_{T_{D^+}} \quad , \end{aligned} \quad (2.29)$$

$$\begin{aligned} \frac{\partial T_{D_2^+}}{\partial t} = & -\frac{1}{B}[\phi, T_{D_2^+}] - v_{\parallel D_2^+} \nabla_{\parallel} T_{D_2^+} - \frac{4}{3} \frac{T_{D_2^+}}{eB} \left[\frac{1}{n_{D_2^+}} C(p_{D_2^+}) + eC(\phi) \right] \\ & - \frac{10}{3} \frac{T_{D_2^+}}{eB} C(T_{D_2^+}) - \frac{2T_{D_2^+}}{3} \nabla_{\parallel} v_{\parallel D_2^+} + \frac{0.92\sqrt{2m_e m_{D_2^+}}}{3} \frac{\sigma_{\parallel}}{en_{D^+}} \nabla_{\parallel} (n_e T_{D^+} \nabla_{\parallel} T_{D^+}) \\ & + \chi_{\perp D_2^+} \nabla_{\perp}^2 T_{D_2^+} + \nabla_{\parallel} (\chi_{\parallel D_2^+} \nabla_{\parallel} T_{D_2^+}) + s_{T_{D_2^+}} \quad , \end{aligned} \quad (2.30)$$

solved together with the Poisson and Ampère equations:

$$\nabla \cdot \left[(n_{D^+} + 2n_{D_2^+}) \nabla_{\perp} \phi \right] = \Omega - \frac{1}{e} \nabla_{\perp}^2 (p_{D^+} + 2p_{D_2^+}) \quad , \quad (2.31)$$

$$\left(\nabla_{\perp}^2 - \frac{e^2 \mu_0}{m_e} n_e \right) v_{\parallel e} = \nabla_{\perp}^2 U_{\parallel e} - \frac{e^2 \mu_0}{m_e} n_{D^+} v_{\parallel D^+} + \frac{e^2 \mu_0}{m_e} j_{\parallel} \quad . \quad (2.32)$$

In Eqs (2.22-2.32), $U_{\parallel e} = V_{\parallel e} + e\psi/m_e$ is the sum of electron inertia and electromagnetic induction, $p_i = n_i T_i$ is the pressure for each species and $\Omega = \Omega_{D^+} + 2\Omega_{D_2^+}$ is the plasma vorticity, where the single species contribute is $\Omega_i = \nabla \cdot \omega_i = \nabla \cdot (n_i \nabla_{\perp} \phi + \nabla_{\perp} p_i)$. The operator $[\phi, f] = \mathbf{b} \cdot (\nabla \phi \times \nabla f)$ is the $\mathbf{E} \times \mathbf{B}$ convective operator, $C(f) = B/2[\nabla \times (\mathbf{b}/B)] \cdot \nabla f$ is the curvature operator and $\nabla_{\perp}^2 f = \nabla \cdot [(\mathbf{b} \times \nabla f) \times \mathbf{b}]$ is the perpendicular Laplacian. The electrical conductivity and parallel conductivities are [60]:

$$\begin{aligned} \sigma_{\parallel} &= 1.96 \frac{n_e e^2 \tau_e}{m_e} \quad , \\ \chi_{\parallel e} &= 3.2 \frac{n_e T_e \tau_e}{m_e} \quad , \\ \chi_{\parallel i} &= 3.9 \frac{n_i T_i \tau_i}{m_i} \quad , \end{aligned} \quad (2.33)$$

for each ion species $i = D^+$ or D_2^+ .

2.2.2 Plasma-neutral collisions

In this section we will describe the interactions between charged species and D and D₂ neutrals considered in our system. For each reaction we will add a contribute to the Boltzmann kinetic equations Eq. (2.1) and derive the source and sink terms appearing in Eqs. (2.22-2.30).

We remark that D₂ molecules can be injected or they can be generated by association of atoms at the vessel walls or by recombination in the plasma volume. Neutral molecules can then be ionized, generating D₂⁺ ions, or undergoing dissociation, producing D⁺ or D. In addition to these processes there will also be electron-neutral collisions, considered elastic, and charge-exchange collisions between ion and neutral species.

The plasma-neutrals interaction considered in our model are listed in Table 2.1. We denote with v_e , v_{D^+} and $v_{D_2^+}$ the modulus of the particle velocities, while σ denotes the reaction cross section for each process. The reaction rates are evaluated considering Krook collision operators, averaging the reaction rates $v\sigma$ over the electron distribution function, effectively neglecting the velocity of the charged or neutral particle involved in the process. In the charge-exchange processes there is weak dependence of the cross section by the ion-neutral relative velocity [12], so the rate is evaluated neglecting the velocity of the neutral particle.

The dependence of the rates $\langle v\sigma \rangle$ by plasma density and temperature is obtained from the AMJUEL [61] and HYDEL [62] databases (see [37] for the detailed reference). In figure 2.1 the rates as a function of the energy of the colliding particle.

Table 2.1: Collisional processes considered and their respective reaction rates.

Collisional process	Equation	Reaction Frequency
Ionization of D	$e^- + D \rightarrow 2e^- + D^+$	$\nu_{iz,D} = n_e \langle v_e \sigma_{iz,D}(v_e) \rangle$
Recombination of D ⁺ and e ⁻	$e^- + D^+ \rightarrow D$	$\nu_{rec,D^+} = n_e \langle v_e \sigma_{rec,D^+}(v_e) \rangle$
e ⁻ - D ⁺ elastic collisions	$e^- + D^+ \rightarrow e^- + D^+$	$\nu_{e-D} = n_e \langle v_e \sigma_{e-D}(v_e) \rangle$
Ionization of D ₂	$e^- + D_2 \rightarrow 2e^- + D_2^+$	$\nu_{iz,D_2} = n_e \langle v_e \sigma_{iz,D_2}(v_e) \rangle$
Recombination of D ₂ ⁺ and e ⁻	$e^- + D_2^+ \rightarrow D_2$	$\nu_{rec,D_2^+} = n_e \langle v_e \sigma_{rec,D_2^+}(v_e) \rangle$
e ⁻ - D ₂ ⁺ elastic collisions	$e^- + D_2^+ \rightarrow e^- + D_2^+$	$\nu_{e-D_2} = n_e \langle v_e \sigma_{e-D_2}(v_e) \rangle$
Dissociation of D ₂	$e^- + D_2 \rightarrow e^- + D + D$	$\nu_{diss,D_2} = n_e \langle v_e \sigma_{diss,D_2}(v_e) \rangle$
Dissociative ionization of D ₂	$e^- + D_2 \rightarrow 2e^- + D^+ + D$	$\nu_{diss-iz,D_2} = n_e \langle v_e \sigma_{diss-iz,D_2}(v_e) \rangle$
Dissociation of D ₂ ⁺	$e^- + D_2^+ \rightarrow e^- + D^+ + D$	$\nu_{diss,D_2^+} = n_e \langle v_e \sigma_{diss,D_2^+}(v_e) \rangle$
Dissociative ionization of D ₂ ⁺	$e^- + D_2^+ \rightarrow 2e^- + 2D^+$	$\nu_{diss-iz,D_2^+} = n_e \langle v_e \sigma_{diss-iz,D_2^+}(v_e) \rangle$
Dissociative recombination of D ₂ ⁺	$e^- + D_2^+ \rightarrow 2D$	$\nu_{diss-rec,D_2^+} = n_e \langle v_e \sigma_{diss-rec,D_2^+}(v_e) \rangle$
Charge-exchange of D ⁺ , D	$D^+ + D \rightarrow D + D^+$	$\nu_{cx,D} = n_{D^+} \langle v_{D^+} \sigma_{cx,D^+}(v_{D^+}) \rangle$
Charge-exchange of D ₂ ⁺ , D ₂	$D_2^+ + D_2 \rightarrow D_2 + D_2^+$	$\nu_{cx,D_2} = n_{D_2^+} \langle v_{D_2^+} \sigma_{cx,D_2^+}(v_{D_2^+}) \rangle$
Charge-exchange of D ₂ ⁺ , D	$D_2^+ + D \rightarrow D_2 + D^+$	$\nu_{cx,D-D_2^+} = n_{D_2^+} \langle v_{D_2^+} \sigma_{cx,D-D_2^+}(v_{D_2^+}) \rangle$
Charge-exchange of D ₂ , D ⁺	$D_2 + D^+ \rightarrow D_2^+ + D$	$\nu_{cx,D_2-D^+} = n_{D^+} \langle v_{D^+} \sigma_{cx,D_2-D^+}(v_{D^+}) \rangle$

Velocities and energies of particles produced in the reactions are evaluated through momentum and energy considerations, resulting in the values listed in Table 2.2 [37]. In charge-exchange processes the sum of the energy of the incoming neutral and ion is assumed to be conserved, while the outgoing particle keeps the incoming velocity. For example,

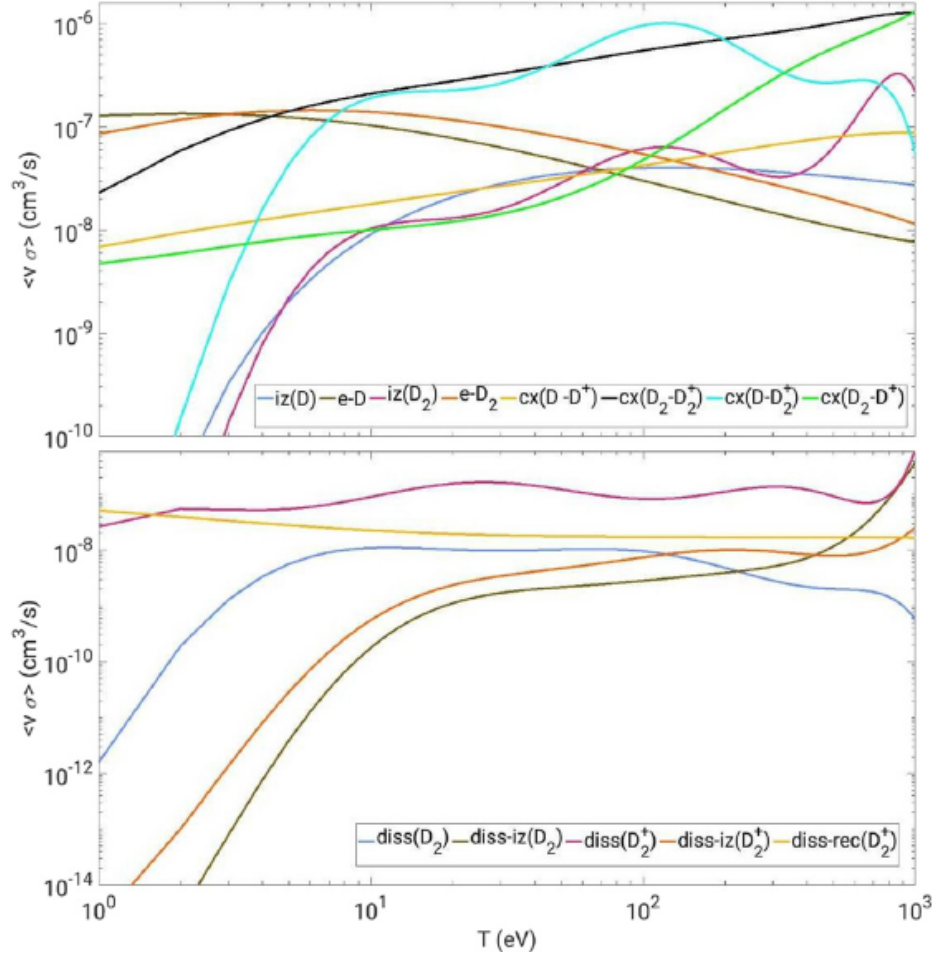


Figure 2.1: Reaction rates $\langle v\sigma \rangle$ for the interactions considered in the model, as a function of the colliding particle energy, taken from [37].

in $D_2^+ + D \rightarrow D_2 + D^+$ the outgoing D_2 will keep the velocity of the D_2^+ and the D^+ will have the same velocity of the D . For elastic collisions between electrons and atomic or molecular neutrals, it is assumed that the neutral velocity is not affected by the reaction, while the electron is emitted isotropically according to a Maxwellian distribution function centered at the velocity of the incoming neutral. For example, for $e - D$ collisions it will be $\Phi_{e[\mathbf{v}_D, T_{e,e-D}]} = [m_e/(2\pi T_{e,e-D})]^{3/2} \exp -m_e(\mathbf{v} - \mathbf{v}_D)^2/(2T_{e,e-D})$, while the electron temperature $T_{e,e-D}$ is evaluated applying the energy conservation between incoming and outgoing particles $3/2T_e + m_e v_e^2/2 = T_{e,e-D} + m_e v_D^2/2$. In D ionization, the outgoing electrons are described by the Maxwellian distribution function $\Phi_{e[\mathbf{v}_D, T_{e-iz(D)}]}$, centered at the fluid velocity of the incoming neutral, where the electron temperature takes into account the ionization energy loss $3/2T_e + m_e v_e^2/2 = 2[T_{e,iz(D)} + m_e v_D^2/2] + \langle E_{iz,D} \rangle$. Ionization of D_2 and dissociation of D_2 and D_2^+ are treated analogously, with specific energy losses, $\langle E_{iz,D_2} \rangle$, $\langle E_{diss,D_2} \rangle$ and $\langle E_{diss,D_2^+} \rangle$, and electron temperatures $T_{e,iz(D_2)}$, $T_{e,diss(D_2)}$ and $T_{e,diss(D_2^+)}$. Dissociative ionization of D_2 generates two electrons, with Maxwellian distribution $\Phi_{e[\mathbf{v}_{D_2}, T_{e,diss-iz(D_2)}]}$, where the temperature satisfies $3/2T_e + m_e v_e^2/2 = 2[T_{e,diss-iz(D_2)} + m_e v_{D_2}^2/2] + \langle E_{diss-iz,D_2} \rangle$. The same is considered for dissociative ionization of D_2^+ . For the atoms D and ions D^+ generated by dissociation processes we assume always Maxwellian distributions, with the same velocity of the incoming molecule and temperatures listed in table 2.2. In particular, the processes are modelled as Franck-Condon collisions [62], where the energy needed to excite the D_2 or D_2^+ is treated as average electron energy loss.

Table 2.2: Average electron energy loss and average energy of reaction products for the ionization and dissociative processes included in the model.

Collisional process	e^- Energy loss	Temperature of products
Ionization of D	$\langle E_{iz,D} \rangle = 13.60\text{eV}$	
Ionization of D_2	$\langle E_{iz,D_2} \rangle = 15.43\text{eV}$	
Dissociation of D_2	$\langle E_{diss,D_2} \rangle \simeq 14.3\text{eV}$	$T_{D,diss(D_2)} \simeq 1.95\text{eV}$
Dissociative ionization of D_2 ($E_e < 26\text{eV}$)	$\langle E_{diss-iz,D_2} \rangle \simeq 18.25\text{eV}$	$T_{D,diss-iz(D_2)} \simeq 0.25\text{eV}$
Dissociative ionization of D_2 ($E_e > 26\text{eV}$)	$\langle E_{diss-iz,D_2} \rangle \simeq 33.6\text{eV}$	$T_{D,diss-iz(D_2)} \simeq 7.8\text{eV}$
Dissociation of D_2^+	$\langle E_{diss,D_2^+} \rangle \simeq 13.7\text{eV}$	$T_{D,diss(D_2^+)} \simeq 3.0\text{eV}$
Dissociative ionization of D_2^+	$\langle E_{diss-iz,D_2^+} \rangle \simeq 15.5\text{eV}$	$T_{D,diss-iz(D_2^+)} \simeq 0.4\text{eV}$
Dissociative recombination of D_2^+		$T_{D,diss-rec(D_2^+)} \simeq 11.7\text{eV}$

The distribution functions of the particles generated by neutral collisions are added to the right hand side of the

Boltzmann kinetic equations Eq. (2.1), where C_n for the considered reactions is

$$\begin{aligned}
 C_n(f_e) = & \nu_{iz,D} n_D \left[2\Phi_{e[\mathbf{v}_D, T_{e,iz(D)}}] - \frac{f_e}{n_e} \right] + \nu_{e-D} n_D \left[\Phi_{e[\mathbf{v}_D, T_{e,en(D)}}] - \frac{f_e}{n_e} \right] \\
 & - \nu_{rec,D^+} \frac{n_{D^+}}{n_e} f_e + \nu_{iz,D_2} n_{D_2} \left[2\Phi_{e[\mathbf{v}_{D_2}, T_{e,iz(D_2)}}] - \frac{f_e}{n_e} \right] \\
 & + \nu_{e-D_2} n_{D_2} \left[\Phi_{e[\mathbf{v}_{D_2}, T_{e,en(D_2)}}] - \frac{f_e}{n_e} \right] - \nu_{rec,D_2^+} \frac{n_{D_2^+}}{n_e} f_e \\
 & + \nu_{diss,D_2} n_{D_2} \left[\Phi_{e[\mathbf{v}_{D_2}, T_{e,diss(D_2)}}] - \frac{f_e}{n_e} \right] + \nu_{diss-iz,D_2} n_{D_2} \left[2\Phi_{e[\mathbf{v}_{D_2}, T_{e,diss-iz(D_2)}}] - \frac{f_e}{n_e} \right] \\
 & + \nu_{diss-iz,D_2^+} n_{D_2^+} \left[2\Phi_{e[\mathbf{v}_{D_2^+}, T_{e,diss-iz(D_2^+)}}] - \frac{f_e}{n_e} \right] \\
 & + \nu_{diss,D_2^+} n_{D_2^+} \left[\Phi_{e[\mathbf{v}_{D_2^+}, T_{e,diss(D_2^+)}}] - \frac{f_e}{n_e} \right] - \nu_{diss-rec,D_2^+} n_{D_2^+} \frac{f_e}{n_e},
 \end{aligned} \tag{2.34}$$

$$\begin{aligned}
 C_n(f_{D^+}) = & \nu_{iz,D} f_D - \nu_{rec,D^+} f_{D^+} \\
 & - \nu_{cx,D} \left(\frac{n_D}{n_{D^+}} f_{D^+} - f_D \right) + \nu_{cx,D-D_2^+} f_D - \nu_{cx,D_2-D^+} \frac{n_{D_2}}{n_{D^+}} f_{D^+} \\
 & + \nu_{diss-iz,D_2} f_{D_2} + 2\nu_{diss-iz,D_2^+} f_{D_2^+} + \nu_{diss,D_2^+} f_{D_2^+},
 \end{aligned} \tag{2.35}$$

$$\begin{aligned}
 C_n(f_{D_2^+}) = & \nu_{iz,D_2} f_{D_2} - \nu_{rec,D_2^+} f_{D_2^+} \\
 & - \nu_{cx,D_2} \left(\frac{n_{D_2}}{n_{D_2^+}} f_{D_2^+} - f_{D_2} \right) - \nu_{cx,D_2-D^+} f_{D_2} - \nu_{cx,D-D_2^+} \frac{n_D}{n_{D_2^+}} f_{D_2^+} \\
 & - \left(\nu_{diss-iz,D_2^+} + \nu_{diss,D_2^+} + \nu_{diss-rec,D_2^+} \right) f_{D_2^+}.
 \end{aligned} \tag{2.36}$$

It is now possible to evaluate all the neutral interactions contributes in Eqs. (2.6-2.13) taking the first three moments of these terms.

Following the same procedure described before to apply the drift approximation, we can now write the friction drift appearing in the ions perpendicular velocities as

$$\begin{aligned}
 \mathbf{v}_{fric,D^+} = & \frac{n_D}{n_{D^+}} \frac{\nu_{cx,D} + \nu_{iz,D} + \nu_{cx,D-D_2^+}}{\Omega_{cD^+}} (\mathbf{v}_{\perp D} - \mathbf{v}_{\perp D^+0}) \times \mathbf{b} + \frac{n_{D_2}}{n_{D^+}} \frac{\nu_{diss-iz,D_2}}{\Omega_{cD^+}} (\mathbf{v}_{\perp D_2} - \mathbf{v}_{\perp D^+0}) \times \mathbf{b} \\
 & \frac{n_{D_2^+}}{n_{D^+}} \frac{2\nu_{diss-iz,D_2^+} + \nu_{diss,D_2^+}}{\Omega_{cD^+}} (\mathbf{v}_{\perp D_2^+} - \mathbf{v}_{\perp D^+0}) \times \mathbf{b},
 \end{aligned} \tag{2.37}$$

$$\mathbf{v}_{fric,D_2^+} = \frac{n_{D_2}}{n_{D_2^+}} \frac{\nu_{iz,D_2} + \nu_{cx,D_2} + \nu_{cx,D_2-D^+}}{\Omega_{cD_2^+}} (\mathbf{v}_{\perp D_2} - \mathbf{v}_{\perp D_2^+0}) \times \mathbf{b}. \tag{2.38}$$

The contribute from the friction drifts, as well as the density and temperature sources and sinks arising from the neutral collisions, are shown in the full set of equations implemented in GBS in the next section, Eqs. (2.39-2.47).

2.2.3 Implementation of the plasma model

The set of equations Eqs. (2.22-2.30), with the neutral interaction terms derived from Eqs. (2.34-2.36), is implemented in GBS in dimensionless form. In the following we will treat the fields that describe the plasma and neutrals as dimensionless:

$$\begin{aligned} \frac{\partial n_e}{\partial t} = & -\frac{\rho_*^{-1}}{B} [\phi, n_e] + \frac{2}{B} [C(p_e) - n_e C(\phi)] - \nabla_{\parallel} (n_e v_{\parallel e}) + \mathcal{D}_{n_e} \nabla_{\perp}^2 n_e + S_{n_e} \\ & + n_D \nu_{iz,D} - n_{D^+} \nu_{rec,D^+} + n_{D_2} \nu_{iz,D_2} - n_{D_2^+} \nu_{rec,D_2^+} \end{aligned} \quad (2.39)$$

$$\begin{aligned} \frac{\partial n_{D_2^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B} [\phi, n_{D_2^+}] - \nabla_{\parallel} (n_{D_2^+} v_{\parallel D_2^+}) - \frac{2}{B} [C(p_{D_2^+}) + n_{D_2^+} C(\phi)] \\ & + \mathcal{D}_{n_{D_2^+}} \nabla_{\perp}^2 n_{D_2^+} + S_{n_{D_2^+}} + n_{D_2} \nu_{iz,D_2} - n_{D_2^+} \nu_{rec,D_2^+} + n_{D_2^+} \nu_{cx,D_2-D^+} \\ & - n_{D^+} \nu_{cx,D-D_2^+} - n_{D_2^+} \left(\nu_{diss-iz,D_2^+} + \nu_{diss,D_2^+} + \nu_{diss-rec,D_2^+} \right) \end{aligned} \quad (2.40)$$

$$\begin{aligned} \frac{\partial \Omega}{\partial t} = & -\frac{\rho_*^{-1}}{B} \nabla \cdot \left([\phi, \omega_{D^+}] + 2 [\phi, \omega_{D_2^+}] \right) - \nabla \cdot \left(v_{\parallel D^+} \nabla_{\parallel} \omega_{D^+} + v_{\parallel D_2^+} \nabla_{\parallel} \omega_{D_2^+} \right) \\ & + 2BC(p_e + p_{D^+} + p_{D_2^+}) + B^2 \nabla_{\parallel} j_{\parallel} + \frac{B}{3} C(G_{D^+} + G_{D_2^+}) \\ & + \eta_{0\Omega} \nabla_{\parallel}^2 \Omega + \mathcal{D}_{\perp \Omega} \nabla_{\perp}^2 \Omega - \nabla \cdot \left[\frac{2n_{D_2}}{n_{D_2^+}} (\nu_{cx,D_2} + \nu_{iz,D_2} + \nu_{cx,D_2-D^+}) \omega_{D_2^+} \right] \end{aligned} \quad (2.41)$$

$$\begin{aligned} \frac{\partial U_{\parallel e}}{\partial t} = & -\frac{\rho_*^{-1}}{B} [\phi, v_{\parallel e}] + \frac{m_{D^+}}{m_e} \left[\nu j_{\parallel} + \nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_e}{n_e} - \frac{2}{3n_e} \nabla_{\parallel} G_e - 0.71 \nabla_{\parallel} T_e \right] \\ & - v_{\parallel e} \nabla_{\parallel} v_{\parallel e} + \mathcal{D}_{v_{\parallel e}} \nabla_{\perp}^2 v_{\parallel e} + \frac{1}{n_e} [n_{D^+} (2\nu_{iz,D} + \nu_{e-D}) (v_{\parallel D^+} - v_{\parallel e}) \\ & + n_{D_2} (2\nu_{iz,D_2} + \nu_{e-D_2} + 2\nu_{diss-iz,D_2} + \nu_{diss,D_2}) (v_{\parallel D_2} - v_{\parallel e}) \\ & + n_{D_2^+} (2\nu_{diss-iz,D_2^+} + \nu_{diss,D_2^+}) (v_{\parallel D_2^+} - v_{\parallel e})] \end{aligned} \quad (2.42)$$

$$\begin{aligned} \frac{\partial v_{\parallel D^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B} [\phi, v_{\parallel D^+}] - v_{\parallel D^+} \nabla_{\parallel} v_{\parallel D^+} - \nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_{D^+}}{n_{D^+}} \\ & - \frac{2}{3n_{D^+}} \nabla_{\parallel} G_{D^+} + 0.71 \frac{n_e}{n_{D^+}} \nabla_{\parallel} T_e - \nu \frac{n_e}{n_{D^+}} j_{\parallel} + \mathcal{D}_{v_{\parallel D^+}} \nabla_{\perp}^2 v_{\parallel D^+} \\ & + \frac{1}{n_{D^+}} [n_D (\nu_{iz,D} + \nu_{cx,D} + \nu_{cx,D-D_2^+}) (v_{\parallel D^+} - v_{\parallel D^+}) \\ & + n_{D_2^+} (2\nu_{diss-iz,D_2^+} + \nu_{diss,D_2^+}) (v_{\parallel D_2^+} - v_{\parallel D^+}) \\ & + n_{D_2} \nu_{diss-iz,D_2} (v_{\parallel D_2} - v_{\parallel D^+})] \end{aligned} \quad (2.43)$$

$$\begin{aligned} \frac{\partial v_{\parallel D_2^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B} [\phi, v_{\parallel D_2^+}] - v_{\parallel D_2^+} \nabla_{\parallel} v_{\parallel D_2^+} + \frac{1}{2} \left[-\nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_{D_2^+}}{n_{D_2^+}} - \frac{2}{3n_{D_2^+}} \nabla_{\parallel} G_{D_2^+} \right] \\ & + \mathcal{D}_{v_{\parallel D_2^+}} \nabla_{\perp}^2 v_{\parallel D_2^+} + \frac{n_{D_2}}{n_{D_2^+}} (\nu_{iz,D_2} + \nu_{cx,D_2} + \nu_{cx,D_2-D^+}) (v_{\parallel D_2^+} - v_{\parallel D_2^+}) \end{aligned} \quad (2.44)$$

$$\begin{aligned}
 \frac{\partial T_e}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, T_e] - v_{\parallel e} \nabla_{\parallel} T_e + \frac{4T_e}{3B} \left[\frac{7}{2} C(T_e) + \frac{T_e}{n_e} C(n_e) - C(\phi) \right] - \frac{2T_e}{3} \nabla_{\parallel} v_{\parallel e} \\
 & + \frac{2}{3n_e} \left[\frac{1.62}{\nu} \nabla_{\parallel} (n_e T_e \nabla_{\parallel} T_e) - 0.71 \nabla_{\parallel} (T_e j_{\parallel}) \right] \\
 & + \mathcal{D}_{\perp e} \nabla_{\perp}^2 T_e + \nabla_{\parallel} (\chi_{\parallel e} \nabla_{\parallel} T_e) + S_{T_e} \\
 & + \frac{1}{n_e} \{ n_D \nu_{iz,D} \left[-\frac{2}{3} E_{iz,D} - T_e + \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - \frac{4}{3} v_{\parallel D^+} \right) \right] \\
 & + n_{D_2} \nu_{iz,D_2} \left[-\frac{2}{3} E_{iz,D_2} - T_e + \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - \frac{4}{3} v_{\parallel D_2^+} \right) \right] \\
 & + n_{D_2} \nu_{diss,D_2} \left[-\frac{2}{3} E_{diss,D_2} + \frac{2}{3} \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - v_{\parallel D_2^+} \right) \right] \\
 & + n_{D_2} \nu_{diss-iz,D_2} \left[-\frac{2}{3} E_{diss-iz,D_2} - T_e + \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - \frac{4}{3} v_{\parallel D_2^+} \right) \right] \\
 & + n_{D_2^+} \nu_{diss,D_2^+} \left[-\frac{2}{3} E_{diss,D_2^+} + \frac{2}{3} \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - v_{\parallel D_2^+} \right) \right] \\
 & + n_{D_2^+} \nu_{diss-iz,D_2^+} \left[-\frac{2}{3} E_{diss-iz,D_2^+} - T_e + \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - \frac{4}{3} v_{\parallel D_2^+} \right) \right] \\
 & - n_{D^+} \nu_{e-D} \frac{m_e}{m_{D^+}} \frac{2}{3} v_{\parallel e} (v_{\parallel D^+} - v_{\parallel e}) - n_{D_2^+} \nu_{e-D_2} \frac{m_e}{m_{D^+}} \frac{2}{3} v_{\parallel e} (v_{\parallel D_2^+} - v_{\parallel e}) \} \quad ,
 \end{aligned} \tag{2.45}$$

$$\begin{aligned}
 \frac{\partial T_{D^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, T_{D^+}] - v_{\parallel D^+} \nabla_{\parallel} T_{D^+} + \frac{4}{3} \frac{T_{D^+}}{B} \left[\frac{1}{n_{D^+}} C(p_e + p_{D_2^+}) - C(\phi) \right] \\
 & - \frac{2T_{D^+}}{3n_{D^+}} \left[\nabla_{\parallel} (n_e v_{\parallel e}) - \nabla_{\parallel} (n_{D_2^+} v_{\parallel D_2^+}) - v_{\parallel D^+} \nabla_{\parallel} (n_{D_2^+}) \right] \\
 & - \frac{10}{3} \frac{T_{D^+}}{B} C(T_{D^+}) + \frac{2}{3n_{D^+}} \frac{2.32}{\sqrt{2\nu}} \sqrt{\frac{m_e}{m_{D^+}}} \nabla_{\parallel} (n_e T_{D^+} \nabla_{\parallel} T_{D^+}) \\
 & + \mathcal{D}_{\perp D^+} \nabla_{\perp}^2 T_{D^+} + \nabla_{\parallel} (\chi_{\parallel D^+} \nabla_{\parallel} T_{D^+}) + S_{T_{D^+}} \\
 & + \frac{1}{n_{D^+}} \left\{ n_D (\nu_{iz,D} + \nu_{cx,D} + \nu_{cx,D-D_2^+}) \left[T_D - T_{D^+} + \frac{1}{3} (v_{\parallel D} - v_{\parallel D^+})^2 \right] \right. \\
 & + n_{D_2} \nu_{diss-iz,D_2} \left[T_{D,diss-iz(D_2)} - T_{D^+} + \frac{1}{3} (v_{\parallel D_2} - v_{\parallel D^+})^2 \right] \\
 & + 2n_{D_2^+} \nu_{diss-iz,D_2^+} \left[T_{D,diss-iz(D_2^+)} - T_{D^+} + \frac{1}{3} (v_{\parallel D_2^+} - v_{\parallel D^+})^2 \right] \\
 & \left. + n_{D_2^+} \nu_{diss,D_2^+} \left[T_{D,diss(D_2^+)} - T_{D^+} + \frac{1}{3} (v_{\parallel D_2^+} - v_{\parallel D^+})^2 \right] \right\} \quad ,
 \end{aligned} \tag{2.46}$$

$$\begin{aligned}
 \frac{\partial T_{D_2^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, T_{D_2^+}] - v_{\parallel D_2^+} \nabla_{\parallel} T_{D_2^+} - \frac{4}{3} \frac{T_{D_2^+}}{B} \left[\frac{1}{n_{D_2^+}} C(p_{D_2^+}) + C(\phi) \right] \\
 & - \frac{10}{3} \frac{T_{D_2^+}}{B} C(T_{D_2^+}) - \frac{2T_{D_2^+}}{3} \nabla_{\parallel} v_{\parallel D_2^+} + \frac{2}{3n_{D_2^+}} \frac{0.92}{\sqrt{2\nu}} \sqrt{\frac{m_e}{m_{D^+}}} \nabla_{\parallel} (n_e T_{D^+} \nabla_{\parallel} T_{D^+}) \\
 & + \mathcal{D}_{\perp D_2^+} \nabla_{\perp}^2 T_{D_2^+} + \nabla_{\parallel} (\chi_{\parallel D_2^+} \nabla_{\parallel} T_{D_2^+}) + S_{T_{D_2^+}} \\
 & + \frac{n_{D_2}}{n_{D_2^+}} (\nu_{cx,D_2} + \nu_{iz,D_2} + \nu_{cx,D_2-D^+}) \left[T_{D_2} - T_{D_2^+} + \frac{2}{3} (v_{\parallel D_2} - v_{\parallel D_2^+})^2 \right] \quad ,
 \end{aligned} \tag{2.47}$$

solved with the Poisson and Ampère equations:

$$\nabla \cdot \left[\left(n_{D^+} + 2n_{D_2^+} \right) \nabla_{\perp} \phi \right] = \Omega - \tau \nabla_{\perp}^2 \left(p_{D^+} + 2p_{D_2^+} \right) , \quad (2.48)$$

$$\left(\nabla_{\perp}^2 - \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} n_e \right) v_{\parallel e} = \nabla_{\perp}^2 U_{\parallel e} - \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} n_{D^+} v_{\parallel D^+} + \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} \bar{j}_{\parallel} , \quad (2.49)$$

while the atomic ions density is evaluated imposing quasi-neutrality $n_{D^+} = n_e - n_{D_2^+}$.

We remark that in Eqs. (2.39-2.49), $U_{\parallel e} = V_{\parallel e} + \frac{m_{D^+}}{m_e} \psi$ is the sum of electron inertia and electromagnetic induction, $p_i = n_i T_i$ is the pressure for each species and $\Omega = \Omega_{D^+} + 2\Omega_{D_2^+}$ is the plasma vorticity, where the single species contribute is $\Omega_i = \nabla \cdot \omega_i = \nabla \cdot (n_i \nabla_{\perp} \phi + \nabla_{\perp} p_i)$. All quantities are normalized to their reference value, in order to be dimensionless. Densities are normalized to the reference density n_0 , electron temperature to T_{e0} , both ion temperatures to T_{D^+0} and velocities to the sound speed $c_{s0} = \sqrt{T_{e0}/m_{D^+}}$. The norm of the magnetic field B is normalized to the field value on the magnetic axis B_0 , perpendicular lengths to the ion sound Larmor radius $\rho_{s0} = c_{s0}/\Omega_{D^+}$, where $\Omega_{D^+} = eB_0/m_{D^+}$, parallel lengths to the tokamak major radius R_0 , and time to $t_0 = R_0/c_{s0}$. The system dynamics is then regulated by dimensionless parameters: the normalized ion Larmor radius, $\rho_* = \rho_{s0}/R_0$, the ion to electron temperature ratio, $\tau = T_{D^+0}/T_{e0}$, and the normalized Spitzer resistivity $\nu = e^2 n_0 R_0 / (m_{D^+} c_{s0} \sigma_{\parallel}) = \nu_0 T_e^{-3/2}$, with

$$\sigma_{\parallel} = \left(1.96 \frac{n_0 e^2 \tau_e}{m_e} \right) n = \left(\frac{5.88}{4\sqrt{2}\pi} \frac{(4\pi\epsilon_0)^2}{e^2} \frac{T_{e0}^{3/2}}{\lambda \sqrt{m_e}} \right) (T_e)^{3/2} \quad (2.50)$$

$$\nu_0 = \frac{4\sqrt{2}\pi}{5.88} \frac{e^4}{(4\pi\epsilon_0)^2} \frac{\sqrt{m_e} R_0 n_0 \lambda}{m_{D^+} c_{s0} T_{e0}^{3/2}} . \quad (2.51)$$

The normalized viscosities are taken as constant, evaluated using the reference density and temperature: $\eta_{0e} = 0.73 n_0 T_{e0} \tau_e$ and $\eta_{0i} = 0.96 n_0 T_{e0} \tau_e$. Thermal conductivities are functions of electron and ions temperatures

$$\begin{aligned} \chi_{\parallel e} &= \left(\frac{1.58}{\sqrt{2}\pi} \frac{m_{D^+}}{\sqrt{m_e}} \frac{(4\pi\epsilon_0)^2}{e^4} \frac{c_{s0}}{R_0} \frac{T_{e0}^{3/2}}{\lambda n_0} \right) T_e^{5/2} \\ \chi_{\parallel i} &= \left(\frac{1.94}{\sqrt{2}\pi} \sqrt{m_i} \frac{(4\pi\epsilon_0)^2}{e^4} \frac{c_{s0}}{R_0} \frac{T_{e0}^{3/2} \tau^{5/2}}{\lambda n_0} \right) T_i^{5/2} , \end{aligned} \quad (2.52)$$

where $i = D^+$ or D_2^+ . The normalized diffusion coefficients D_f , for each field f , are introduced for numerical stability.

In our simulations, fuelling is entirely the result of neutral ionization processes, while external electron heating is added in Eq. (2.45) as s_{T_e} , a source toroidally uniform expressed as an analytical function of the flux function

$$s_{T_e} = \frac{s_{T0}}{2} \left[\tanh \left(-\frac{\psi(R, Z) - \psi_T}{\Delta_T} \right) + 1 \right] , \quad (2.53)$$

where ψ_T is a flux surface localized inside the LCFS. The resulting heating source in the model is the sum of the contributes given by heating and by neutral interactions in Eqs. (2.39-2.47)

$$s_{P_{\text{tot}}} = n_e (s_{T_e} + s_{T_e}^{\text{neu}}) + n_{D^+} s_{T_{D^+}}^{\text{neu}} + n_{D_2^+} s_{T_{D_2^+}}^{\text{neu}} + T_e s_{n_e}^{\text{neu}} + T_{D^+} s_{n_{D^+}}^{\text{neu}} + T_{D_2^+} s_{n_{D_2^+}}^{\text{neu}} . \quad (2.54)$$

The simulation domain encompasses the whole tokamak plasma volume, with a rectangular poloidal cross section of vertical extension L_Z and radial extension L_R , leading to a natural choice of a cylindrical coordinate system (R, φ, Z) , where R is the radial distance from the tokamak axis of symmetry, φ the toroidal angle and Z the vertical coordinate. The magnetic field is expressed in terms of the flux function ψ , $\mathbf{B} = RB_\varphi \nabla \varphi + \nabla \psi \times \nabla \varphi$, where $\nabla \psi$ is the direction orthogonal to the flux surface, defining a flux aligned coordinate system used in the analysis $(\nabla \psi, \nabla \chi, \nabla \varphi)$, where $\nabla \chi = \nabla \varphi \times \nabla \psi$. The differential operators in the cylindrical coordinate system, in normalized units, become $[\phi, f] = \frac{B_\varphi}{B}(\partial_Z \phi \partial_R f - \partial_R \phi \partial_Z f)$, $C(f) = \frac{B_\varphi}{B} \partial_Z f$, $\nabla_{\parallel} f = \partial_Z \Psi \partial_R f - \partial_R \Psi \partial_Z f + \frac{B_\varphi}{B} \partial_\varphi f$ and $\nabla_{\perp}^2 f = \partial_{RR}^2 f + \partial_{ZZ}^2 f$.

All plasma quantities are evaluated on a uniform Cartesian grid that discretizes the R , Z and φ coordinates. The spatial operators are discretized by a fourth-order centered finite difference scheme, utilizing a 5-points stencil for first derivatives. The grid for densities, temperatures and ϕ are evaluated on a grid staggered in the Z and φ direction with respect to the grid for $v_{\parallel e}$, $v_{\parallel D^+}$, $v_{\parallel D_2^+}$, in order to avoid the formation of numerical checkerboard patterns with centered schemes [63]. The Poisson brackets are instead discretized by means of a fourth-order Arakawa scheme [64]. The time evolution is provided by a fourth-order Runge-Kutta algorithm.

2.2.4 Boundary conditions

Close to the vessel walls, inside the magnetic pre-sheath, the drift approximation used to derive the model equations is violated by the presence of a large electric field. Therefore, the boundary conditions applied in GBS are evaluated at the entrance of the magnetic pre-sheath. The generalized Bohm-Chodura set of magnetic conditions was first derived in [65], then improved in [51]. The extension of the pre-sheath set of magnetic boundary conditions for molecular deuterium is detailed in [37]. It follows the same approach used in [65] and [51], considering strong gradients at the boundary, neglecting finite Larmor radius effects and assuming $n_{D_2^+}/n_e \ll 1$. The result is

$$v_{\parallel e} = \pm c_s \max\left\{\exp\left(\Lambda - \frac{\phi}{T_e}\right), \exp(\Lambda)\right\} \quad (2.55)$$

$$v_{\parallel D^+} = \pm c_s \sqrt{1 + \frac{T_{D^+}}{T_e}} \quad (2.56)$$

$$v_{\parallel D_2^+} = \frac{v_{\parallel D^+}}{\sqrt{2}} \quad (2.57)$$

$$\partial_n \phi = \mp \frac{c_s}{\sqrt{1 + \frac{T_{D^+}}{T_e}}} \partial_n v_{\parallel D^+} \quad (2.58)$$

$$\partial_n n_e = \mp \frac{n_e}{c_s \sqrt{1 + \frac{T_{D^+}}{T_e}}} \partial_n v_{\parallel D^+} \quad (2.59)$$

$$\partial_n n_{D^+} = \partial_n n_e \quad (2.60)$$

$$\partial_n n_{D_2^+} = \mp \frac{n_{D_2^+}}{c_s \sqrt{1 + \frac{T_{D^+}}{T_e}}} \partial_n v_{\parallel D^+} \quad (2.61)$$

$$\partial_n T_e = \partial_n T_{D^+} = \partial_n T_{D_2^+} = 0 \quad (2.62)$$

$$\Omega = \mp (n_e + n_{D_2^+}) \sqrt{1 + \frac{T_i}{T_e}} \partial_{nn}^2 v_{\parallel D^+} \quad (2.63)$$

where n is the normal to the boundary, the plus (minus) sign refers to the case of the magnetic field pointing toward (away) from it, the dimensionless ion sound speed is $c_s = \sqrt{T_e}$ and $\Lambda = \log \sqrt{m_{D^+}/(2\pi m_e)} \simeq 3$ for deuterium plasma. A set of simplified boundary conditions is also used where the ion flux to the wall is lower, e.g. where there are no strike points, with $\phi = \Lambda T_e$, implying $v_{\parallel e} = \pm c_s$.

2.3 The kinetic neutral model

The neutral model used in this work is based on a kinetic description of the neutral dynamics, in order to avoid restriction on the neutrals mean free path $\lambda_{\text{mfp,D}}$, and it is resolved without using a Monte Carlo method, in order to avoid statistical noise. Its resolution was first presented in [36] for the case of a mono-atomic neutral species, then extended in [37] for the case of molecular deuterium and implemented in a limited version of GBS. In this section will be followed the same approach, solving the neutral dynamics that will be coupled to the plasma model described in Sec. 2.2 and ultimately allowing the simulation of molecular reactions in diverted configuration. It's important to underline that the model solution will be given for molecular deuterium, but it can be applied to any other species.

2.3.1 Formal solution of the multi-species model

The starting point is the set of two kinetic Boltzmann equations, for D and D₂, that characterize the evolution of the two distribution functions f_D and f_{D_2} , with the reactions considered in table 2.1:

$$\begin{aligned} \frac{\partial f_D}{\partial t} + \mathbf{v} \cdot \frac{\partial f_D}{\partial \mathbf{x}} = & -\nu_{\text{iz,D}} f_D - \nu_{\text{cx,D}} \left(f_D - \frac{n_D}{n_{D^+}} f_{D^+} \right) + \nu_{\text{rec,D}^+} f_{D^+} \\ & + \nu_{\text{cx,D}_2\text{-D}^+} \left(\frac{n_{D_2}}{n_{D^+}} f_{D^+} \right) - \nu_{\text{cx,D-D}_2^+} f_D + 2\nu_{\text{diss,D}_2} f_{D_2} + \nu_{\text{diss-iz,D}_2} f_{D_2} \\ & + \nu_{\text{diss,D}_2^+} f_{D_2^+} + 2\nu_{\text{diss-rec,D}_2^+} f_{D_2^+} , \end{aligned} \quad (2.64)$$

$$\begin{aligned} \frac{\partial f_{D_2}}{\partial t} + \mathbf{v} \cdot \frac{\partial f_{D_2}}{\partial \mathbf{x}} = & -\nu_{\text{iz,D}_2} f_{D_2} - \nu_{\text{cx,D}_2} \left(f_{D_2} - \frac{n_{D_2}}{n_{D_2^+}} f_{D_2^+} \right) + \nu_{\text{rec,D}_2^+} f_{D_2^+} - \nu_{\text{cx,D}_2\text{-D}^+} f_{D_2} \\ & + \nu_{\text{cx,D-D}_2^+} \left(\frac{n_D}{n_{D_2^+}} f_{D_2^+} \right) - \nu_{\text{diss,D}_2} f_{D_2} - \nu_{\text{diss-iz,D}_2} f_{D_2} , \end{aligned} \quad (2.65)$$

where all the reaction frequencies ν are defined in table 2.1.

Once the plasma quantities are known, the formal solution of Eqs. (2.64-2.65) can be found applying the method of characteristics, yielding:

$$\begin{aligned} f_n(\mathbf{x}, \mathbf{v}, t) = & \int_0^{r'_b} \left[\frac{S_n(\mathbf{x}', \mathbf{v}, t')}{v} + \delta(r' - r'_b) f_n(\mathbf{x}'_b, \mathbf{v}, t'_b) \right] \\ & \times \exp \left[-\frac{1}{v} \int_0^{r'} \nu_{\text{eff},n}(\mathbf{x}'', t'') dr'' \right] dr' , \end{aligned} \quad (2.66)$$

for each neutral species $n = \text{D}$ or D_2 . Eq. (2.66) describes the distribution function of neutrals at position $\mathbf{x}$, velocity $\mathbf{v}$ and time t , as the result of neutrals generated at position $\mathbf{x}' = \mathbf{x} - r' \mathbf{v}/v$, and time $t' = t - r'/v$, where r' is

the coordinate along the characteristic connecting $\mathbf{x}'$ and $\mathbf{x}$, and r'_b denotes the distance between the point $\mathbf{x}$ and the intersection of the characteristic with the boundary. The terms S_n are the volumetric source of D or D₂, written as

$$\begin{aligned}
 S_D(\mathbf{x}', \mathbf{v}, t') = & \nu_{\text{cx},D}(\mathbf{x}', t') n_D(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D^+}, T_{D^+}]}(\mathbf{x}', \mathbf{v}, t') + \nu_{\text{cx},D_2-D^+}(\mathbf{x}', t') n_D(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D^+}, T_{D^+}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + \nu_{\text{rec},D^+}(\mathbf{x}', t') n_{D^+}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D^+}, T_{D^+}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + 2\nu_{\text{diss},D_2}(\mathbf{x}', t') n_{D_2}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2}, T_{D,\text{diss}(D_2)}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + \nu_{\text{diss-iz},D_2}(\mathbf{x}', t') n_{D_2}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2}, T_{D,\text{diss-iz}(D_2)}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + \nu_{\text{diss},D_2^+}(\mathbf{x}', t') n_{D_2^+}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2}, T_{D,\text{diss}(D_2^+)}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + 2\nu_{\text{diss-rec},D_2^+}(\mathbf{x}', t') n_{D_2^+}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2^+}, T_{D,\text{diss-rec}(D_2^+)}]}(\mathbf{x}', \mathbf{v}, t') \quad ,
 \end{aligned} \tag{2.67}$$

$$\begin{aligned}
 S_{D_2}(\mathbf{x}', \mathbf{v}, t') = & \nu_{\text{cx},D_2}(\mathbf{x}', t') n_{D_2}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2^+}, T_{D_2^+}]}(\mathbf{x}', \mathbf{v}, t') + \nu_{\text{cx},D-D_2^+}(\mathbf{x}', t') n_D(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2^+}, T_{D_2^+}]}(\mathbf{x}', \mathbf{v}, t') \\
 & + \nu_{\text{rec},D_2^+}(\mathbf{x}', t') n_{D_2^+}(\mathbf{x}', t') \Phi_{[\mathbf{v}_{D_2^+}, T_{D_2^+}]}(\mathbf{x}', \mathbf{v}, t') \quad ,
 \end{aligned} \tag{2.68}$$

where the ions distribution functions Φ are taken as Maxwellian distributions and the energies of the products is computed as described in section 2.2.2. The ions velocity $\mathbf{v}_{D^+}$ and $\mathbf{v}_{D_2^+}$ is evaluated considering the leading order components as described in Sec. 2.2, neglecting $\mathbf{v}_{D_2}$ and $\mathbf{v}_{D_2^+}$ with respect to $\mathbf{v}_{D^+}$.

The exponential term in Eq. (2.66) describes the sink due to the sum of any reaction that removes neutrals from the system, with

$$\nu_{\text{eff},D}(\mathbf{x}'', t'') = \nu_{\text{iz},D}(\mathbf{x}'', t'') + \nu_{\text{cx},D}(\mathbf{x}'', t'') + \nu_{\text{cx},D-D_2^+}(\mathbf{x}'', t'') \quad , \tag{2.69}$$

$$\begin{aligned}
 \nu_{\text{eff},D_2}(\mathbf{x}'', t'') = & \nu_{\text{iz},D_2}(\mathbf{x}'', t'') + \nu_{\text{cx},D_2}(\mathbf{x}'', t'') + \nu_{\text{cx},D_2-D^+}(\mathbf{x}'', t'') \\
 & + \nu_{\text{diss},D_2}(\mathbf{x}'', t'') + \nu_{\text{diss-iz},D_2}(\mathbf{x}'', t'') \quad .
 \end{aligned} \tag{2.70}$$

The remaining contribute to neutrals emission, D or D₂, is caused by the outflowing ion flux, D⁺ or D₂⁺, on the tokamak vessel. The boundary condition for the distribution function, $f_n(\mathbf{x}_b, \mathbf{v}, t'_b)$ in Eq. (2.66), is chosen to describe recycling and associative processes at the wall. A fraction of the ion flux, α_{refl} , is reflected as fast neutrals, with the same temperature of the impacting ion, while the remaining flux is absorbed by the wall and emitted with the boundary temperature T_b . In a similar way, we consider also the contribute to neutral emission of reflection or re-emission by the same neutral species flux. In addition, a small fraction β_{assoc} of the D⁺ flux recombines with electrons and D, contributing to the D₂ emission. The resulting boundary condition for D is:

$$\begin{aligned}
 f_D(\mathbf{x}'_b, \mathbf{v}, t') = & (1 - \alpha_{\text{refl}}) \Gamma_{\text{emiss},D}(\mathbf{x}'_b, t') \chi_{\text{in},D}(\mathbf{x}'_b, \mathbf{v}, T_b) \\
 & + \alpha_{\text{refl}} [f_D(\mathbf{x}'_b, \mathbf{v} - 2\mathbf{v}_p, t') + f_{D^+}(\mathbf{x}'_b, \mathbf{v} - 2\mathbf{v}_p, t')] \quad ,
 \end{aligned} \tag{2.71}$$

where $\chi_{\text{in},D}$ is the emitted neutral velocity distribution and $|\mathbf{v}_p| = \mathbf{v} \cdot \hat{\mathbf{n}}$ is the velocity in the direction perpendicular to the wall. For the D₂ species we impose an equivalent boundary condition. The neutrals emitted from the wall are

proportional to the outgoing flux of neutrals and ions, including the probability of undergo association:

$$\Gamma_{\text{emiss,D}}(\mathbf{x}'_b) = (1 - \beta_{\text{assoc}}) (\Gamma_{\text{out,D}}(\mathbf{x}'_b) + \Gamma_{\text{out,D}^+}(\mathbf{x}'_b)) \quad (2.72)$$

$$\Gamma_{\text{emiss,D}_2}(\mathbf{x}'_b) = \Gamma_{\text{out,D}_2}(\mathbf{x}'_b) + \Gamma_{\text{out,D}_2^+}(\mathbf{x}'_b) + \frac{\beta_{\text{assoc}}}{2} (\Gamma_{\text{out,D}}(\mathbf{x}'_b) + \Gamma_{\text{out,D}^+}(\mathbf{x}'_b)) \quad , \quad (2.73)$$

where in the ions flux it is considered the projection of the sum of the parallel flux and the diamagnetic and $\mathbf{E} \times \mathbf{B}$ drifts, e.g. for D^+ $\Gamma_{\text{out,D}^+} = n_{\text{D}^+} [v_{\parallel \text{D}^+} \cdot \mathbf{b} + v_{\mathbf{E} \times \mathbf{B}} + v_{\text{dD}^+}] \cdot \hat{\mathbf{n}}$, and in the neutral flux it is considered the flux directed toward the boundary, e.g. $\Gamma_{\text{out,D}} = - \int_{v_p < 0} (\mathbf{v}_p \cdot \mathbf{n}) f_{\text{D}} d\mathbf{v}$. The velocity distribution function for neutrals emitted by the wall follows a Knudsen cosine law $\chi_{\text{in,D}} = 3/(4\pi) m_{\text{D}}^2 / T_b^2 \cos(\theta) \exp(-(m_{\text{D}} v^2)/(2T_b))$, and equivalently for D_2 , with $\theta = \arccos(v_p/v)$ angle between the $\mathbf{v}$ and the perpendicular to the wall.

Following the procedure in [36, 37], the integral equation in Eq. (2.66) can be simplified considering that the typical neutral time of flight is shorter than the turbulent timescales $\tau_n \ll \tau_{\text{turb}}$, equivalent to consider $t' = t$, thus neglecting the time dependence. It is also safe to assume that the neutral mean free path is typically smaller than the length of the turbulence, i.e. $\lambda_{\text{mfp},n} k_{\parallel} \ll 1$ for $n = \text{D}$ or D_2 , reducing the system to a two-dimensional plane, that coincides with the poloidal plane of our plasma model. Considering the integral of Eq. (2.66) in velocity space, it's possible to retrieve an equation for neutral densities, where the time and parallel coordinate dependence are only parametric. Finally, the set of equations will be

$$\begin{aligned} n_{\text{D}}(\mathbf{x}_{\perp}) = & \int_{\text{S}} n_{\text{D}}(\mathbf{x}'_{\perp}) \nu_{\text{cx,D}}(\mathbf{x}'_{\perp}) K_{p \rightarrow p}^{\text{D,D}^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{cx,D}_2\text{-D}^+}(\mathbf{x}'_{\perp}) K_{p \rightarrow p}^{\text{D,D}^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} 2n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{diss,D}_2}(\mathbf{x}'_{\perp}) K_{p \rightarrow p}^{\text{D,diss}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{diss-iz,D}_2}(\mathbf{x}'_{\perp}) K_{p \rightarrow p}^{\text{D,diss-iz}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\partial \text{S}} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) (1 - \beta_{\text{assoc}}) \Gamma_{\text{out,D}}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow p}^{\text{D,reem}}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp,b}) da'_b \\ & + n_{\text{D}[\text{rec}(\text{D}^+)]}(\mathbf{x}_{\perp}) + n_{\text{D}[\text{out}(\text{D}^+)]}(\mathbf{x}_{\perp}) + n_{\text{D}[\text{diss}(\text{D}_2^+)]}(\mathbf{x}_{\perp}) \quad , \end{aligned} \quad (2.74)$$

$$\begin{aligned} \Gamma_{\text{out,D}}(\mathbf{x}_{\perp,b}) = & \int_{\text{S}} n_{\text{D}}(\mathbf{x}'_{\perp}) \nu_{\text{cx,D}}(\mathbf{x}'_{\perp}) K_{p \rightarrow b}^{\text{D,D}^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{cx,D}_2\text{-D}^+}(\mathbf{x}'_{\perp}) K_{p \rightarrow b}^{\text{D,D}^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} 2n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{diss,D}_2}(\mathbf{x}'_{\perp}) K_{p \rightarrow b}^{\text{D,diss}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\text{S}} n_{\text{D}_2}(\mathbf{x}'_{\perp}) \nu_{\text{diss-iz,D}_2}(\mathbf{x}'_{\perp}) K_{p \rightarrow b}^{\text{D,diss-iz}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) dA' \\ & + \int_{\partial \text{S}} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) (1 - \beta_{\text{assoc}}) \Gamma_{\text{out,D}}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow b}^{\text{D,reem}}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp,b}) da'_b \\ & + \Gamma_{\text{D}[\text{rec}(\text{D}^+)]}(\mathbf{x}_{\perp}) + \Gamma_{\text{D}[\text{out}(\text{D}^+)]}(\mathbf{x}_{\perp}) + \Gamma_{\text{D}[\text{diss}(\text{D}_2^+)]}(\mathbf{x}_{\perp}) \quad , \end{aligned} \quad (2.75)$$

$$\begin{aligned}
 n_{D_2}(\mathbf{x}_\perp) = & \int_S n_{D_2}(\mathbf{x}'_\perp) \nu_{cx,D_2}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \\
 & + \int_{\partial S} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) \Gamma_{\text{out}, D_2}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow p}^{D_2}(\mathbf{x}_\perp, \mathbf{x}'_{\perp,b}) da'_b \\
 & + \int_{\partial S} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) \frac{\beta_{\text{assoc}}}{2} \Gamma_{\text{out}, D}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow p}^{D_2}(\mathbf{x}_\perp, \mathbf{x}'_{\perp,b}) da'_b \\
 & + \int_S n_D(\mathbf{x}'_\perp) \nu_{cx, D-D_2^+}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \\
 & + n_{D_2[\text{rec}(D_2^+)]}(\mathbf{x}_\perp) + n_{D_2[\text{out}(D_2^+)]}(\mathbf{x}_\perp) + n_{D_2[\text{out}(D^+)]}(\mathbf{x}_\perp) \quad ,
 \end{aligned} \tag{2.76}$$

$$\begin{aligned}
 \Gamma_{\text{out}, D_2}(\mathbf{x}_{\perp,b}) = & \int_S n_{D_2}(\mathbf{x}'_\perp) \nu_{cx,D_2}(\mathbf{x}'_\perp) K_{p \rightarrow b}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \\
 & + \int_{\partial S} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) \Gamma_{\text{out}, D_2}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow b}^{D_2}(\mathbf{x}_\perp, \mathbf{x}'_{\perp,b}) da'_b \\
 & + \int_{\partial S} (1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp,b})) \frac{\beta_{\text{assoc}}}{2} \Gamma_{\text{out}, D}(\mathbf{x}'_{\perp,b}) K_{b \rightarrow b}^{D_2}(\mathbf{x}_\perp, \mathbf{x}'_{\perp,b}) da'_b \\
 & + \int_S n_D(\mathbf{x}'_\perp) \nu_{cx, D-D_2^+}(\mathbf{x}'_\perp) K_{p \rightarrow b}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \\
 & + \Gamma_{\text{out}, D_2[\text{rec}(D_2^+)]}(\mathbf{x}_\perp) + \Gamma_{\text{out}, D_2[\text{out}(D_2^+)]}(\mathbf{x}_\perp) + \Gamma_{\text{out}, D_2[\text{out}(D^+)]}(\mathbf{x}_\perp) \quad ,
 \end{aligned} \tag{2.77}$$

where the integral is carried out over the surface of each poloidal plane S or over its boundary ∂S .

In Eqs. (2.74-2.77) the terms $K_{i \rightarrow j}$ are kernel functions, where it is included the integral in neutral velocity space, with the velocity distribution given by the different neutral production processes. They are defined between the location of the source $\mathbf{x}'_\perp$ and target $\mathbf{x}_\perp$, where both of them could be inside the plasma volume p , or on the boundary b . Each kernel function is defined as

$$K_{i \rightarrow j}(\mathbf{x}_\perp, \mathbf{x}'_\perp) = K_{i \rightarrow j, \text{dir}}(\mathbf{x}_\perp, \mathbf{x}'_\perp) + \alpha_{\text{refl}} K_{i \rightarrow j, \text{refl}}(\mathbf{x}_\perp, \mathbf{x}'_\perp) , \tag{2.78}$$

where two contributes are considered: one from the path connecting directly $\mathbf{x}'_\perp$ and $\mathbf{x}_\perp$ and one from the path that connects them through one reflection on the wall. The domain considered is the full tokamak volume, without holes, with four walls, resulting in five possible paths connecting each couple of point inside the plasma volume. For a chosen path, the typical shape of one kernel function is like the one appearing in eq. (2.79):

$$K_{p \rightarrow p, \text{path}}^{D, D^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) = \int_0^\infty \frac{1}{r'_{\text{path}}} \Phi_{\perp[\mathbf{v}_{\perp D^+}, T_{D^+}]}(\mathbf{x}'_\perp, \mathbf{v}_\perp) \exp \left[\frac{1}{v_\perp} \int_0^{r'_{\perp, \text{path}}} \nu_{\text{eff}, D}(\mathbf{x}''_\perp) dr'' \right] dv_\perp \quad , \tag{2.79}$$

where $\text{path} = \text{dir}, \text{refl}$, $r'_{\perp, \text{path}}$ is the distance between $\mathbf{x}_\perp$ and $\mathbf{x}'_\perp$ along the considered path and the velocity distribution $\Phi_{\perp[\mathbf{v}_{\perp D^+}, T_{D^+}]}(\mathbf{x}'_\perp, \mathbf{v}_\perp) = \int_{-\infty}^\infty \Phi_{[\mathbf{v}_{\perp D^+}, T_{D^+}]}(\mathbf{x}'_\perp, \mathbf{v}_\perp) dv_\parallel$. The detailed expression for each kernel function appearing in Eqs. (2.79-2.73) is reported in the appendix.

The contribute to the neutral densities and fluxes that do not depend directly on neutrals can be evaluated separately for each process. For the atomic neutral density there will be a contribute by volumetric recombination, one by

recombination at the boundary wall and one by dissociation of D_2^+ , written as

$$n_{D[\text{rec}(D^+)]}(\mathbf{x}_\perp) = \int_S n_{D^+}(\mathbf{x}'_\perp) \nu_{\text{rec}, D^+}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D, D^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \quad , \quad (2.80)$$

$$n_{D[\text{out}(D^+)]} = \int_{\partial S} \Gamma_{\text{out}, D^+}(\mathbf{x}'_{\perp, b}) [(1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp, b})) (1 - \beta_{\text{assoc}}) K_{b \rightarrow p}^{D, \text{reem}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp, b}) + \alpha_{\text{refl}} K_{b \rightarrow p}^{D, \text{refl}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp, b})] da'_b \quad (2.81)$$

$$n_{D[\text{diss}(D_2^+)]} = \int_S n_{D_2^+}(\mathbf{x}'_\perp) [\nu_{\text{diss}, D_2^+}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D, \text{diss}(D_2^+)}(\mathbf{x}_\perp, \mathbf{x}'_\perp) + 2\nu_{\text{diss-rec}, D_2^+}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D, \text{diss-rec}(D_2^+)}(\mathbf{x}_\perp, \mathbf{x}'_\perp)] dA' \quad . \quad (2.82)$$

For the molecular neutral density there will be a contribute from volumetric recombination, one from recombination at the walls and one from association of D^+ :

$$n_{D_2[\text{rec}(D_2^+)]}(\mathbf{x}_\perp) = \int_S n_{D_2^+}(\mathbf{x}'_\perp) \nu_{\text{rec}, D_2^+}(\mathbf{x}'_\perp) K_{p \rightarrow p}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) dA' \quad , \quad (2.83)$$

$$n_{D_2[\text{out}(D_2^+)]} = \int_{\partial S} \Gamma_{\text{out}, D_2^+}(\mathbf{x}'_{\perp, b}) [(1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp, b})) K_{b \rightarrow p}^{D_2, \text{reem}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp, b}) + \alpha_{\text{refl}} K_{b \rightarrow p}^{D_2, \text{refl}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp, b})] da'_b \quad (2.84)$$

$$n_{D_2[\text{out}(D^+)]} = \int_{\partial S} \Gamma_{\text{out}, D^+}(\mathbf{x}'_{\perp, b}) [(1 - \alpha_{\text{refl}}(\mathbf{x}'_{\perp, b})) \frac{\beta_{\text{assoc}}}{2} K_{b \rightarrow p}^{D_2, \text{reem}}(\mathbf{x}_\perp, \mathbf{x}'_{\perp, b})] da'_b \quad . \quad (2.85)$$

An equivalent contribute to the ones in Eqs. (2.80-2.85) can be found for Γ_D and Γ_{D_2} , for target points on the boundary of our domain.

The model foresees the possibility of a D or D_2 gas puff, modelled as an additional flux from the boundary, directed toward the plasma volume, $\Gamma_{n, \text{puff}}(\mathbf{x}_{\perp, b})$. The contribute of the puff can be evaluated with the same procedure used for the outgoing ion flux, Eq. (2.81) and Eq.(2.84), adding to Eqs. (2.79-2.77) the terms $n_{D[\text{puff}(n)]}$, $\Gamma_{\text{out}, D[\text{puff}(n)]}$, $n_{D_2[\text{puff}(n)]}$, $\Gamma_{\text{out}, D_2[\text{puff}(n)]}$, with $n = D$ or D_2 .

The system of integral equations (2.79) and (2.40) can be solved on a discretized grid, as described in the following section, obtaining the profiles for n_D and n_{D_2} . With them, it is possible to build an equation for any higher-order moment of the neutral quantities. In particular, to solve the set of plasma equations (2.39)-(2.47), it is necessary to evaluate $v_{\parallel n} = 1/n_n \int (\mathbf{v} \cdot \mathbf{b}) f_n d\mathbf{v}$ and $T_n = 1/n_n \int m_n/3 (\mathbf{v} - \bar{\mathbf{v}})^2 f_n d\mathbf{v}$, for $n = D$ and D_2 .

2.3.2 Implementation of the neutral model

To solve the neutral model and find n_D and n_{D_2} , the set of Eqs. (2.79-2.77) is discretized on a linearization of the poloidal plane, where each point represents a set of coordinates (R, Z) . The resulting matrix system is

$$\begin{bmatrix} n_D \\ \Gamma_D \\ n_{D_2} \\ \Gamma_{D_2} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \begin{bmatrix} n_D \\ \Gamma_D \\ n_{D_2} \\ \Gamma_{D_2} \end{bmatrix} + \begin{bmatrix} n_{D[\text{rec}(D^+)]} + n_{D[\text{out}(D^+)]} + n_{D[\text{diss}(D_2^+)]} \\ \Gamma_{\text{out},D[\text{rec}(D^+)]} + \Gamma_{\text{out},D[\text{out}(D^+)]} + \Gamma_{\text{out},D[\text{diss}(D_2^+)]} \\ n_{D_2[\text{rec}(D_2^+)]} + n_{D_2[\text{out}(D_2^+)]} + n_{D[\text{out}(D^+)]} \\ \Gamma_{\text{out},D_2[\text{rec}(D_2^+)]} + \Gamma_{\text{out},D_2[\text{out}(D_2^+)]} + \Gamma_{\text{out},D_2[\text{out}(D^+)]} \end{bmatrix}, \quad (2.86)$$

where the elements M_{ij} are the discretization of the terms in Eqs. (2.79-2.73):

$$\begin{aligned} M_{11} &= \nu_{\text{cx},D} K_{p \rightarrow p}^{\text{D},\text{D}^+}, \\ M_{21} &= \nu_{\text{cx},D} K_{p \rightarrow b}^{\text{D},\text{D}^+}, \\ M_{31} &= \frac{n_{D_2^+}}{n_D} \nu_{\text{cx},D_2^+ - D} K_{p \rightarrow p}^{\text{D}_2,\text{D}_2^+}, \\ M_{41} &= \frac{n_{D_2^+}}{n_D} \nu_{\text{cx},D_2^+ - D} K_{p \rightarrow b}^{\text{D}_2,\text{D}_2^+}, \\ M_{12} &= (1 - \alpha_{\text{refl}})(1 - \beta_{\text{assoc}}) K_{b \rightarrow p}^{\text{D},\text{reem}}, \\ M_{22} &= (1 - \alpha_{\text{refl}})(1 - \beta_{\text{assoc}}) K_{b \rightarrow b}^{\text{D},\text{reem}}, \\ M_{32} &= (1 - \alpha_{\text{refl}}) \frac{\beta_{\text{assoc}}}{2} K_{b \rightarrow p}^{\text{D}_2,\text{reem}}, \\ M_{42} &= (1 - \alpha_{\text{refl}}) \frac{\beta_{\text{assoc}}}{2} K_{b \rightarrow b}^{\text{D}_2,\text{reem}}, \\ M_{13} &= \nu_{\text{cx},D_2 - D^+} K_{p \rightarrow p}^{\text{D},\text{D}^+} + \nu_{\text{diss},D_2} K_{p \rightarrow p}^{\text{D,diss}(D_2)} + \nu_{\text{diss-iz},D_2} K_{p \rightarrow p}^{\text{D,diss-iz}(D_2)}, \\ M_{23} &= \nu_{\text{cx},D_2 - D^+} K_{p \rightarrow b}^{\text{D},\text{D}^+} + \nu_{\text{diss},D_2} K_{p \rightarrow b}^{\text{D,diss}(D_2)} + \nu_{\text{diss-iz},D_2} K_{p \rightarrow b}^{\text{D,diss-iz}(D_2)}, \\ M_{33} &= \nu_{\text{cx},D_2} K_{p \rightarrow p}^{\text{D}_2,\text{D}_2^+}, \\ M_{43} &= \nu_{\text{cx},D_2} K_{p \rightarrow b}^{\text{D}_2,\text{D}_2^+}, \\ M_{14} &= 0, \\ M_{24} &= 0, \\ M_{34} &= (1 - \alpha_{\text{refl}}) K_{b \rightarrow p}^{\text{D}_2}, \\ M_{44} &= (1 - \alpha_{\text{refl}}) K_{b \rightarrow b}^{\text{D}_2}. \end{aligned} \quad (2.87)$$

Each element in the matrix, M_{ij} , contains the information about the path connecting the point P_i and P_j , where P represents a pair of coordinates (R, Z) . The dimension of the matrix is $[2(N_P \times N_B)]^2$, where $N_P = N_R^n \times N_Z^n$ is the number of points that discretize the poloidal plane of the neutrals grid and $N_B = 2(N_R^n + N_Z^n)$ is the number of points used to discretize the boundary. The system in Eq. (2.86) can be solved through the inversion of the matrix $A = (\mathbb{I} - M)$. Due to the absence of holes in the poloidal plane, the matrix A has all non-zero elements and its inversion can be costly. In other works it was observed that the evolution of the neutral dynamics can be evaluated with time steps longer than the time steps used to evolve the plasma [39]. In GBS it is implemented a short-cycling scheme where the neutral profiles are evaluated after multiple plasma steps, usually in the order of hundreds. Recently it was

implemented also the possibility to run plasma and neutral evolution in parallel, on different set of processors [31]. The matrix system is solved using an iterative solver, implemented in the framework provided by the PETSc library with *GMRES* solver without preconditioner. To guarantee the optimal set of neutral's parameters, a set of convergence tests to determine the grid resolution and the time step was also performed and presented in [31].

2.4 Single species reduction

In several GBS studies, e.g. in [66, 31, 67], and also for a part of the work performed for this thesis, see Ch. 3, a deuterium plasma containing a single ion and a single neutral species was modelled. It's important to remark that the set of Eqs. (2.39-2.47) in the special case of $n_{D_2^+} = 0$ and $n_{D_2} = 0$ is reduced to the model of a plasma composed only by electrons, D^+ ions and D neutrals. In particular, $n_e = n_{D^+} = n$ and the Zhdanov closure is reduced to the Braginskii closure presented in [17]. We report here the specific set of equations used in this case:

$$\frac{\partial n}{\partial t} = -\frac{\rho_*^{-1}}{B}[\phi, n] + \frac{2}{B}[C(p_e) - nC(\phi)] - \nabla_{\parallel}(nv_{\parallel e}) + \mathcal{D}_n \nabla_{\perp}^2 n + n_D \nu_{iz,D} - n\nu_{rec,D^+} \quad , \quad (2.88)$$

$$\begin{aligned} \frac{\partial \Omega}{\partial t} = & -\frac{\rho_*^{-1}}{B} \nabla \cdot ([\phi, \omega_{D^+}]) - \nabla \cdot (v_{\parallel D^+} \nabla_{\parallel} \omega_{D^+}) + 2BC(p_e + p_{D^+}) + B^2 \nabla_{\parallel} j_{\parallel} \\ & + \frac{B}{3} C(G_{D^+}) + \eta_{0\Omega} \nabla_{\parallel}^2 \Omega + \mathcal{D}_{\perp \Omega} \nabla_{\perp}^2 \Omega - \frac{n_D}{n} \nu_{cx,D} \Omega \quad , \end{aligned} \quad (2.89)$$

$$\begin{aligned} \frac{\partial U_{\parallel e}}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, v_{\parallel e}] + \frac{m_{D^+}}{m_e} \left[\nu j_{\parallel} + \nabla_{\parallel} \phi - \frac{\nabla_{\parallel} p_e}{n} - \frac{2}{3n} \nabla_{\parallel} G_e - 0.71 \nabla_{\parallel} T_e \right] \\ & - v_{\parallel e} \nabla_{\parallel} v_{\parallel e} + \mathcal{D}_{v_{\parallel e}} \nabla_{\perp}^2 v_{\parallel e} + \frac{n_D}{n} (2\nu_{iz,D} + \nu_{e-D}) (v_{\parallel D^+} - v_{\parallel e}) \quad , \end{aligned} \quad (2.90)$$

$$\begin{aligned} \frac{\partial v_{\parallel D^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, v_{\parallel D^+}] - \frac{1}{n} \nabla_{\parallel} (p_e + \tau p_{D^+}^+) \\ & - \frac{2}{3n} \nabla_{\parallel} G_{D^+} - v_{\parallel D^+} \nabla_{\parallel} v_{\parallel D^+} + \mathcal{D}_{v_{\parallel D^+}} \nabla_{\perp}^2 v_{\parallel D^+} \\ & + \frac{n_D}{n} (\nu_{iz,D} + \nu_{cx,D}) (v_{\parallel D} - v_{\parallel D^+}) \quad , \end{aligned} \quad (2.91)$$

$$\begin{aligned} \frac{\partial T_e}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, T_e] - v_{\parallel e} \nabla_{\parallel} T_e + \frac{4T_e}{3B} \left[\frac{7}{2} C(T_e) + \frac{T_e}{n} C(n) - C(\phi) \right] \\ & - \frac{2T_e}{3} \left[0.71 \frac{\nabla_{\parallel} j_{\parallel}}{n} - \nabla_{\parallel} v_{\parallel e} \right] - 2.61 \nu n (T_e - \tau T_{D^+}) + \mathcal{D}_{\perp e} \nabla_{\perp}^2 T_e \\ & + \nabla_{\parallel} (\chi_{\parallel e} \nabla_{\parallel} T_e) + S_{T_e} + \frac{n_D}{n} \nu_{iz,D} \left[-\frac{2}{3} E_{iz,D} - T_e + \frac{m_e}{m_{D^+}} v_{\parallel e} \left(v_{\parallel e} - \frac{4}{3} v_{\parallel D^+} \right) \right] \quad , \end{aligned} \quad (2.92)$$

$$\begin{aligned} \frac{\partial T_{D^+}}{\partial t} = & -\frac{\rho_*^{-1}}{B}[\phi, T_{D^+}] - v_{\parallel D^+} \nabla_{\parallel} T_{D^+} + \frac{4}{3} \frac{T_{D^+}}{B} \left[\frac{1}{n} C(p_e) - C(\phi) \right] \\ & - \frac{2T_{D^+}}{3} \left[(v_{\parallel D^+} - v_{\parallel e}) \frac{\nabla_{\parallel} n}{n} - \nabla_{\parallel} v_{\parallel e} \right] - \frac{10}{3} \tau \frac{T_{D^+}}{B} C(T_{D^+}) + 2.61 \nu n (T_e - \tau T_{D^+}) \\ & + \mathcal{D}_{\perp D^+} \nabla_{\perp}^2 T_{D^+} + \nabla_{\parallel} (\chi_{\parallel D^+} \nabla_{\parallel} T_{D^+}) + S_{T_{D^+}} \\ & + \frac{n_D}{n} (\nu_{iz,D} + \nu_{cx,D}) \left[T_D - T_{D^+} + \frac{1}{3} (v_{\parallel D} - v_{\parallel D^+})^2 \right] \quad , \end{aligned} \quad (2.93)$$

solved with the Poisson and Ampère equations:

$$\nabla \cdot (n \nabla_{\perp} \phi) = \Omega - \tau \nabla_{\perp}^2 p_{D^+} \quad , \quad (2.94)$$

$$\left(\nabla_{\perp}^2 - \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} n \right) v_{\parallel e} = \nabla_{\perp}^2 U_{\parallel e} - \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} n v_{\parallel D^+} + \frac{\beta_{e0}}{2} \frac{m_{D^+}}{m_e} \bar{j}_{\parallel} \quad , \quad (2.95)$$

where the plasma vorticity for a single species is $\Omega = \Omega_{D^+} = \nabla \cdot \omega_{D^+} = \nabla \cdot (n \nabla_{\perp} \phi + \nabla_{\perp} p_{D^+})$.

In the single neutral species case, also the system in Eq.(2.86) is greatly reduced

$$\begin{bmatrix} n_D \\ \Gamma_D \end{bmatrix} = \begin{bmatrix} \nu_{cx}^{D,D^+} K_{p \rightarrow p}^{D,D^+} & (1 - \alpha_{\text{refl}}) K_{b \rightarrow p}^{D,D^+} \\ \nu_{cx}^{D,D^+} K_{b \rightarrow p}^{D,D^+} & (1 - \alpha_{\text{refl}}) K_{b \rightarrow b}^{D,D^+} \end{bmatrix} \begin{bmatrix} n_D \\ \Gamma_D \end{bmatrix} + \begin{bmatrix} n_{D[\text{rec}(D^+)]} + n_{D[\text{out}(D^+)]} \\ \Gamma_{\text{out},D[\text{rec}(D^+)]} + \Gamma_{\text{out},D[\text{out}(D^+)]} \end{bmatrix} \quad , \quad (2.96)$$

where the size of the matrix is now $(N_P \times N_B)^2$.

2.5 Conclusion

In this chapter we present a multi-component plasma model for the self-consistent description of the neutral and plasma dynamics in the tokamak boundary, which is implemented in the GBS code. A deuterium plasma is modelled in the full tokamak torus, featuring electrons, D^+ and D_2^+ ions, D atoms and D_2 molecules. The multi-component plasma model is based upon the Braginskii fluid equations in the drift-limit [38], with the closure proposed by Zhdanov [58]. The coupling between plasma and neutrals introduces additional terms in the plasma equation, evaluated following the derivation of the Braginskii equations. The considered reactions are D and D_2 ionization, D^+ and D_2^+ recombination, including Molecular Activated Recombination, several charge exchange processes and molecules dissociation. The plasma model is implemented in the latest version of GBS, exploiting the improvements introduced to improve the code efficiency [31]. The neutrals are computed by solving two coupled kinetic equations for the D and D_2 species by using the method of characteristics [39]. In the system neutrals can be generated through ion recycling at the walls or recombination and dissociation reactions in the volume, while ionization is responsible for the losses of D and D_2 particles. The resulting system of linear integral equations are discretized and solved with respect to the densities of neutral species, n_D and n_{D_2} . The system can be then resolved to evaluate higher-order moments of the neutral distribution functions, finding a self-consistent profile for the neutral parallel velocity and the neutral temperature, that will be used in the plasma model equations. The possibility to model molecular plasma in a diverted configuration, without the need of ad-hoc diffusion coefficients and without introducing Monte Carlo noise, will be exploited in Ch. 4 to present the first simulations of turbulence in detachment conditions.

We also introduce the equations used to simulate a single ion species, coupled with a single neutral species with the same mass. This model is equivalent to the five species one, in the peculiar case $n_{D_2} = n_{D_2^+} = 0$. It was already used in several GBS works, e.g. in [31, 68], including the simulations presented in Ch. 3.

We remark that the procedure described in this chapter to derive both plasma and neutral models can be extended to include other species of plasma particles or neutrals, considering the desired collisional processes.

3 Density shoulder investigation

The first analysis proposed with the GBS model presented in Ch. 2 was the study of the density shoulder formation using turbulent simulations. The work was carried out with the first implementation of the model, where only one ion species and one neutral species were considered, i.e. using the model in Sec. 2.4. The main results discussed in this chapter are presented in [68].

3.1 Introduction

Neutrals in the boundary of fusion plasma devices play a crucial role in several phenomena, e.g. providing the power and momentum loss mechanisms needed to reach plasma detachment [69, 70, 71], in the L-H mode transition and in the enhancement of edge plasma turbulence [72], possibly through a reduction of the amplitude of zonal flows [73] or by sustaining filamentary transport thanks to local ionization [74]. The latter two mechanisms have been proposed also as possible candidates for the formation of the *density shoulder*, i.e. the flattening of the scrape-off layer (SOL) density profile at the tokamak outer mid-plane (OMP) observed when core density is increased by increase in fuelling [41].

Even if the formation of the density shoulder is the subject of a number of experimental investigations carried out in several devices [41, 75, 76, 77], there is still debate about the physical mechanisms behind it [76, 78, 79]. As a matter of fact, a proper modelling of plasma-neutrals interactions in a full tokamak turbulent simulation is generally thought necessary to gain the fundamental insights on this phenomenon. Since flatter density profiles are often observed to affect the transport in the SOL and the fluxes to the vessel wall [78, 80], the understanding of the density shoulder formation is of crucial importance for the design of plasma facing components in high-density devices.

In this chapter, the results of the first simulations of GBS in a lower single-null configuration, with the neutral dynamics included, are presented and discussed. As shown in Ch. 2, these simulations leverage recent effort to extend the capabilities of GBS to simulate plasma turbulence in arbitrary magnetic configurations in a full torus, thus retaining the SOL-edge-core interplay [81, 82]. Following [36], neutral dynamics is simulated by considering a single mono-atomic neutral species that interacts with the plasma through ionization, charge-exchange, recombination and elastic electron-neutral collisions. The solution of a kinetic equation for the neutrals allows us to self-consistently simulate the neutral

dynamics, without making assumptions on neutrals transport coefficients as typically required by the fluid approaches [74]. Plasma profiles are evolved without separation between equilibrium and fluctuating quantities, as they result from the self-consistent interplay of the sources of plasma density and heat, perpendicular turbulent transport, parallel flow and losses at the vessels walls.

A scan of simulations is described, with increasing core fuelling, showing that neutrals affect both the plasma profiles and turbulence properties. In particular an increase of the plasma resistivity is observed, associated with an increase of fuelling, leading to an increase of the e-folding length in the near SOL. In the far SOL, an increase of the fuelling rate leads to an increase in plasma density. This result is in agreement with experimental evidences when the density shoulder forms in high-fuelling scenarios. Based on the turbulent transport analysis, a comparison between expected and measured near and far density e-folding length is performed, resulting in good agreement. Associated with the increased density, an increase of the blob size and a decrease in blob radial velocity are observed. On the other hand, by comparing parallel and perpendicular fluxes in the SOL, the increase in far SOL density observed at high fueling is shown to be mainly due to the strong decrease of parallel transport. This is caused by the electron cooling, resulting from ionization reactions in the core and in the SOL region, that reduce the plasma outflow speed to the wall.

After the introduction, in Sec. 3.2 there is an overview of the results obtained from a scan of simulations where we vary the core fuelling. The physical mechanisms behind the formation of the density shoulder are analysed in section 3.3 and the conclusions follow.

3.2 Overview of the simulations

The results described in the present work are based on a set of simulations carried out with the GBS code implementing the model described in Sec. 2.4. All simulations consider the same flux function ψ , which is evaluated from the solution of Biot-Savart law in the infinite aspect-ratio limit for two currents: one centered at the magnetic axis and one outside the domain (see Fig. 3.1), as a matter of fact the same equilibrium used in [82]. Contour levels of the flux function are also shown in figure 3.1. The plasma current on axis is set to have safety factors $q_0 \simeq 1$ at the axis and $q_{95} \simeq 4$ at the edge. In addition, all simulations consider the same geometrical parameters: $L_Z = 800\rho_{s0}$, $L_R = 600\rho_{s0}$, $\rho_*^{-1} = 500$, $a/R_0 = 0.3$. With the choice of $T_{e0} = 20\text{eV}$, if we consider a magnetic field typical of a TCV discharge $B = 0.9T$ and atomic deuterium plasma, composed by D^+ ions, we find the ion sound speed $c_{s0} = 3.8 \times 10^4 \text{m/s}$, the ion sound Larmor radius $\rho_{s0} = 0.5\text{mm}$, $a = 0.076\text{m}$ and $R_0 = 0.254\text{m}$, approximately, 1/3 of the TCV tokamak [83]. Other plasma parameters that are constant throughout the scan are $\tau = 1$, $\eta_{0e} = \eta_{0i} = 1$, $\chi_{||e} = \chi_{||i} = 2$ and $D_f = 16$ for all fields f . In Eqs. (2.92-2.93) the temperature source terms are equal for both species $s_{T_e} = s_{T_{D^+}} = s_T$, where s_T is toroidally uniform and we express it as an analytical function of the flux function

$$s_T = \frac{s_{T0}}{2} \left[\tanh \left(-\frac{\psi(R, Z) - \psi_T}{\Delta_T} \right) + 1 \right] \quad (3.1)$$

where ψ_T is a flux surface localized inside the LCFS, at a position $R - R_{\text{sep}} = -45\rho_{s0}$ at $Z = 0$, as shown in figure 3.1, and Δ_T corresponds to an interval $\Delta R = 40\rho_{s0}$ at $Z = 0$.

In the model we consider the presence of a single neutral species, atomic deuterium D. Regarding the parameters that describe the neutral-plasma interaction, we consider an effective ionization energy of $E_{iz} = 30.0 \text{eV}$, taking into

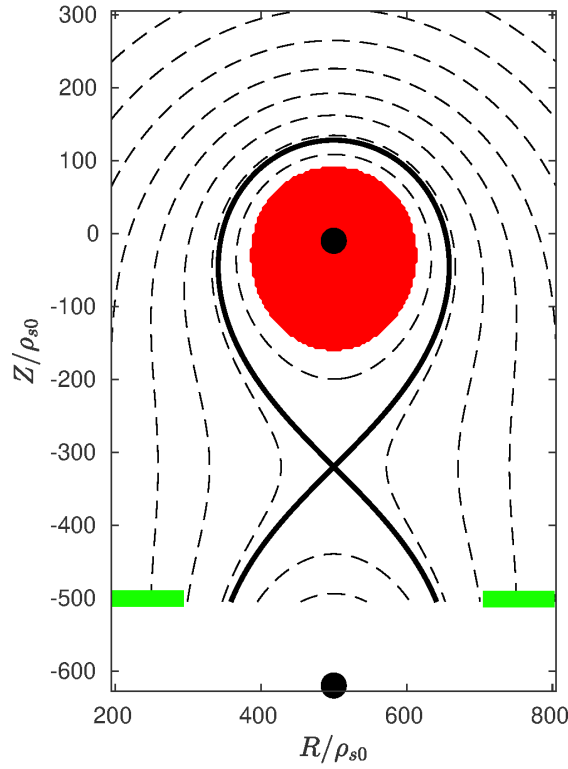


Figure 3.1: Flux surface of ψ function in the domain considered for our simulations. The two black dots represent the position of the current density that generates the magnetic field. The bottom dot is outside the simulation domain. The red region indicate the position of the temperature source, the green lines indicate the pumping regions at the lower boundary of the domain.

account the radiation losses that occur with ionization [12]. Volumetric recombinations and recycling on the left and right walls are neglected, while for all four walls a constant reflection coefficient $\alpha_{\text{refl}} = 0.2$ is considered. The model foresees that all neutrals absorbed by the wall and re-emitted go through a Franck-Condon dissociation process, the emission temperature of the neutrals is then set to $T_b = 3\text{eV}$ [12]. At the bottom-left and bottom-right corners of the rectangular poloidal plane we introduce two neutral pumping regions where neutral emission is suppressed (green line in Fig. 3.1). In addition, to avoid that the density in the private flux region drops to very low values that are detrimental for the numerical stability of the simulations, we use a gas puff that provides a small source of neutrals in this region. This source, which has the same amplitude in all simulations, does not have a relevant impact on the simulation results.

In the scan we control the neutral reaction rates by varying the normalized plasma resistivity ν_0 (see Eq. (2.50)). Then, to have simulations in comparable conditions, the amplitude of the temperature source s_{T0} is adjusted to have the same power outflowing into the SOL for all the three simulations (we choose the value $S_P \simeq (313 \pm 34) \text{ kW}$). The parameters that are varied throughout the simulations are summarized in table 3.1, with the density values being normalized to the same $n_0 = 4 \times 10^{-19} \text{ m}^{-3}$. Since simulations with higher ν_0 show higher fuelling in the core (the terms s_n^{neu} in Eq. (2.54), here $s_{n_e}^{\text{neu}} = s_{n_{D+}}^{\text{neu}} = s_n^{\text{neu}}$), in the following we name the simulations with low, medium and high fuelling as $S_{n,l}$, $S_{n,m}$ and $S_{n,h}$. As discussed later, we compare our simulations with the results of a set of simulations that do not include neutral dynamics, and have the same power source S_P as the simulations with neutrals and same density source, $S_{n,l}$, $S_{n,m}$ and $S_{n,h}$.

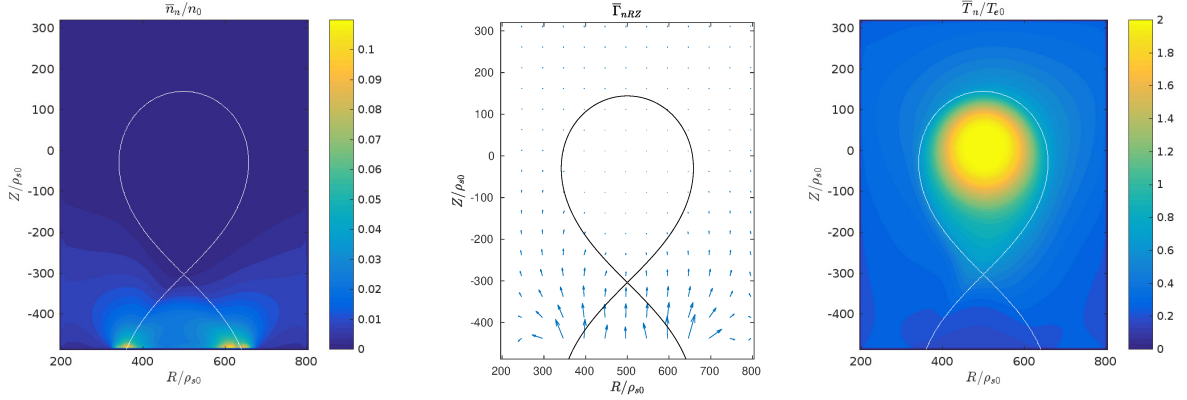


Figure 3.2: Time and toroidally averaged neutral density, $\bar{n}_n/n_0$, neutral flux, $\bar{\Gamma}_{n,RZ}$, and neutral temperature, $\bar{T}_n/T_{e0}$, for the $S_{n,l}$ simulation.

We use a grid $N_R \times N_Z \times N_\phi = 240 \times 320 \times 80$ and a time-step $\Delta t = 3 \times 10^{-5} t_0$ to discretize the plasma equations. The grid for the neutrals is $N_R^n \times N_Z^n \times N_\phi^n = 72 \times 96 \times 80$ and the solution of the neutral model is evaluated every $\Delta t \simeq 0.1 t_0$. The grid used and the neutrals evaluation frequency ensure that our simulation results are converged [31].

After a transient the simulations reach a quasi-steady state where plasma and neutral quantities oscillate around a constant value. In these conditions, the sources, parallel and perpendicular transport and the losses at vessel balance each other. We remark that the parameter chosen for our simulations mimic the typical conditions found in L-mode diverted discharges, as described in [82]. In this regime, turbulent transport is mostly interchange dominated and is characterized by eddies developing near the separatrix, with small or negligible effects due to $E \times B$ shear.

Typical simulations results during this quasi-steady state are shown in Figs. 3.2 and 3.3. All quantities are averaged toroidally and over a $15 t_0$ period (we will denote with tilde fluctuating quantities and with the overline their time average, e.g. $\phi = \tilde{\phi} + \bar{\phi}$). The neutral density, flux and temperature in the poloidal plane are shown in Fig. 3.2 (the $S_{n,l}$ simulation is considered). Neutral density peaks at the bottom wall, near the strike points where most of the ions impact the wall and are recycled. The presence of neutrals is observed both in the private and common flux regions. We point out that the gas puff, positioned at the center of the private flux region, is used only for numerical stability and it does not have an effect on the neutral density profile, like expected. The neutral flux is large near the divertor plates and points toward the core, rapidly decreasing because of the loss of neutrals due to ionizations and the effect of charge-exchange collisions on the neutral velocity. Inside the last-closed flux surface (LCFS), above the X-point, plasma temperature and density are sufficiently high to ionize the remaining neutrals. Neutral temperature is lower at the target walls, where most of the neutrals are created, and has a value close to $T_b = 3\text{eV}$. The temperature increases inside the plasma volume because of charge-exchange reactions, which produce high temperature neutrals. The average plasma density, electron and ion temperatures, the average plasma parallel current and the average electrostatic potential, are shown in Fig. 3.3. These profile are in qualitative agreement with past GBS simulations without neutrals [82, 84], suggesting that the density source used in the simulations without neutral dynamics is able to mimic the self-consistent fuelling that takes place as a consequence of the plasma-neutrals interactions.

The simulations with higher S_n are expected to have, in general, higher reaction rates for the collisions between plasma and neutral particles, through the enhancement of the neutral interaction terms in Eqs. (2.88-2.93), affecting therefore

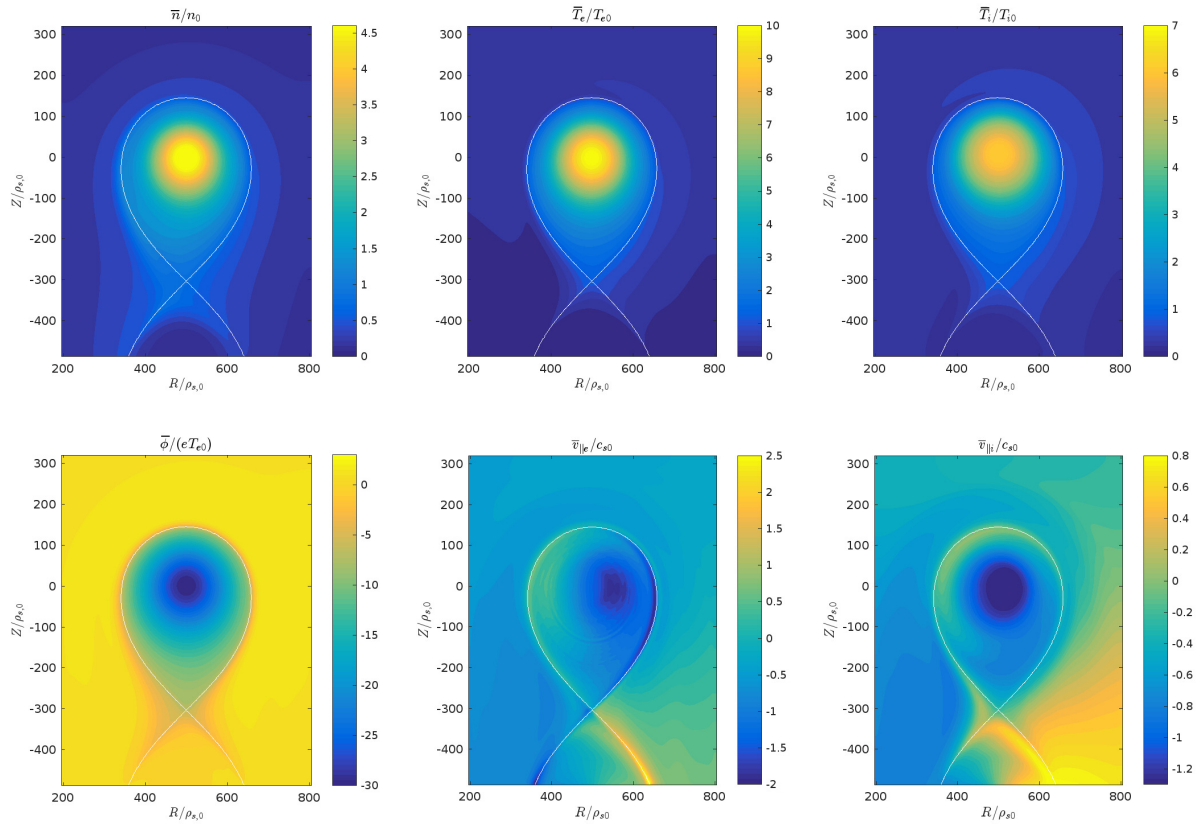


Figure 3.3: Time and toroidally averaged plasma density, $\bar{n}/n_0$, electron temperature, $\bar{T}_e/T_{e0}$, ion temperature, $\bar{T}_i/T_{i0}$, electrostatic potential, $\bar{\phi}/(eT_{e0})$, electron parallel velocity, $\bar{v}_{||e}/c_{s0}$, and ion parallel velocity, $\bar{v}_{||i}/c_{s0}$, for the $S_{n,l}$ simulation.

Table 3.1: Input parameters, ν_0 and s_{T0} , and main results of the three simulations considered in the present paper. All simulations have the same core power source, $S_P \simeq (313 \pm 34)\text{kW}$, while the density source in the core, S_n , is given by ionization reactions. Density values and sources are normalized to the same reference density $n_0 = 4 \times 10^{19} \text{ m}^{-3}$, temperatures to the reference electron temperature $T_{e0} = 20 \text{ eV}$.

Label	ν_0	$s_{T0}/(T_{e0}/t_0)$	$S_n/(n_0\rho_{s0}^2/t_0)$	n_{sep}/n_0	$T_{e,\text{sep}}/T_{e0}$	θ	ν_{sep}	$L_n^{\text{near}}/\rho_{s0}$	$L_n^{\text{far}}/\rho_{s0}$
$S_{n,l}$	0.4	0.16	0.97×10^3	0.47	1.16	0.74	0.81	25.89	186.34
$S_{n,m}$	0.8	0.20	1.10×10^3	0.53	0.97	0.86	1.05	35.66	189.42
$S_{n,h}$	1.6	0.22	1.35×10^3	0.55	0.86	0.90	1.26	65.26	205.27

the simulation results. In fact, higher density source S_n is the result of higher ionization reaction rates, which introduces a temperature sink lowering the temperature in the core and in the SOL, despite the fact that the amplitude of the temperature source, s_{T0} , is increased to keep the power constant throughout the scan. In particular, this leads to an increase in resistivity at the separatrix, $\nu_{\text{sep}} \propto T_{e,\text{sep}}^{-3/2}$ (see table 3.1).

In the present work we focus on the profiles of plasma density and electron pressure at the outer mid-plane (OMP), where for OMP we consider the average over a region of vertical extension $20\rho_{s0}$. In Fig. 3.4 the density and electron pressure profiles are shown for the three simulations considered. The fits of the density and electron pressure reveal two different decay lengths. A steep decay is observed in the near SOL and across the LCFS, with density and pressure decay lengths L_n^{near} and L_{pe}^{near} . A weaker decay is observed further away from the separatrix, in the far SOL, corresponding to lengths L_n^{far} and L_{pe}^{far} . This double decay length is a feature seen both in experiments [76, 85] and simulations [86]. One also observes that the density increases in the far SOL with increasing core fuelling S_n , a property that recalls the formation of the density shoulder seen experimentally [78, 87].

In order to quantify the double scale length structure and its dependence on S_n , we introduce the separatrix density, n_{sep} , and temperature, $T_{e,\text{sep}}$ and define the transition density n_{tr} as the density at the intersection between the exponential fits of the near and far SOL density profile. We also introduce the ratio of the density at the interface between far and near SOL expressed as $\theta = n_{\text{tr}}/n_{\text{sep}}$. When $\theta \simeq 1$ the profile exhibits high density in the far SOL, without a clear separation between near and far SOL. Table 3.1 provides the computed values for all simulations.

Besides the mentioned increase in resistivity at the separatrix, the analysis of the simulation results at the OMP shows that the increase of S_n leads to the increase of θ , and therefore of the far SOL density. Higher fuelling is also associated with a less noticeable increase of L_n^{near} . The increase of the far SOL density and L_n^{near} with ν_{sep} is a feature already observed with GBS [82], but in our simulations the increase in resistivity is the self-consistent result of the increase of neutral ionizations. The far SOL decay length, L_n^{far} , instead shows differences below 15%, suggesting comparable perpendicular flux far from the separatrix, expected to be proportional to the L_n^{far} [84].

3.3 Investigation of the mechanisms behind the density shoulder formation

The plasma profiles in the SOL are the results of the interplay between perpendicular transport of plasma and heat from the core toward the wall, transport along the magnetic field lines to the divertor plates and local interactions with the neutral species.

Enhanced perpendicular transport due to large filaments is currently thought to be one of the main causes for shoulder

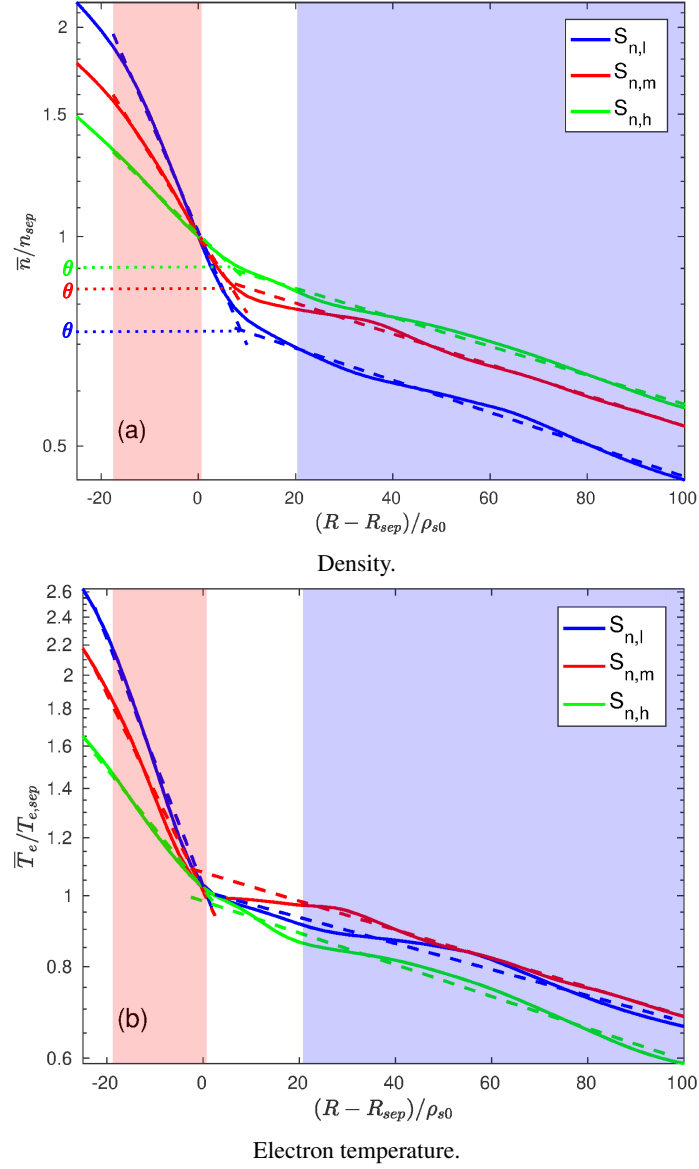


Figure 3.4: Averaged radial profile of density (a) and electron temperature (b) normalized to the value at the separatrix at the OMP. Dashed line represent the exponential fit in the near SOL and in the far SOL. In red shadow the region used for the near SOL fit, in blue the region for the far SOL fit. Pointed line represent the value of $\theta = n_{tr}/n_{sep}$.

formation [41, 78, 88]. Along with this mechanism, two other effects were proposed to have a significant impact in the broadening of the SOL profiles, that is the decrease in parallel transport [77, 89] and the increase in ionization in the OMP [74, 76, 79]. In the following we disentangle the three effects in order to investigate the mechanisms behind the shoulder formation.

While we focus on the density profiles and fluxes in what follows, we note that the flattening of pressure profile is also shown as S_n is increased (see Fig. 3.4). This is despite the fact that the increase of ionizations with S_n is responsible for the decrease of the electron temperature at the separatrix.

3.3.1 Perpendicular transport

We focus on $\bar{\Gamma}_{E \times B}$, the time and toroidally averaged cross-field transport induced by the $E \times B$ drift, since it is significantly larger than the one induced by the diamagnetic drift. In addition, we observe that the contribution of the stationary flow $\bar{n} \partial_\chi \bar{\phi}$ to $\bar{\Gamma}_{E \times B}$ can be neglected, consistently with the general observation that perpendicular transport is mostly driven by turbulence [66]. It is therefore possible to approximate $\bar{\Gamma}_{E \times B} \simeq \bar{n} \partial_\chi \bar{\phi}$.

In Fig. 3.5 we show the radial profiles of $\bar{\Gamma}_{E \times B}$, $\bar{\Gamma}_{E \times B}/|\nabla \bar{n}|$ and $\bar{\Gamma}_{E \times B}/\bar{n}$ at the OMP for the three simulations. We observe that the average of all quantities decrease progressively with the increase of S_n and, therefore, with the plasma resistivity, as opposed to the increase of $\bar{n}$ in the far SOL. In particular, $\bar{\Gamma}_{E \times B}/|\nabla \bar{n}|$ shows that the effective plasma turbulent diffusion coefficient in the far SOL decreases with the increase of S_n . The same result are retrieved from the profile of $\bar{\Gamma}_{E \times B}/\bar{n}$, an estimate of the effective convective transport velocity, that decreases with increasing ionization source. This contrasts, at least in the condition explored in the present set of simulations, with the hypothesis advanced since the first experimental evidences [90, 91], that shoulder formation is due to an enhanced perpendicular transport. As an aside, we note that the diffusivity parameters D_f introduced for numerical stability are one order of magnitude lower than the turbulent transport coefficient shown in Fig. 3.5.

In order to investigate the reason behind the decrease of the transport with S_n , we carry out a detailed investigations of the mechanisms that determine it. Our simulations as well as experimental evidences, show that transport in the far SOL is highly intermittent and associated with the radial motion of coherent filamentary structures denoted as blobs [78, 88, 92, 93, 94]. In Fig. 3.6 a snapshot of the normalized density fluctuations $\tilde{n} = (n - \bar{n})/\bar{n}$ for a specific time and φ , together with the time trace of density for a point in the near SOL and one in the far SOL. On the poloidal plane it's possible to see that turbulent eddies develop mainly in the LFS, growing in the core and moving toward the far SOL. From the time traces we can see the intermittent nature of turbulence, where the peaks in the near SOL are followed by peaks in the far SOL, characteristic of moving structures.

In our simulations, blobs are identified and their motion is studied with an algorithm developed and used for the analysis of previous GBS results [95, 96, 97]. The algorithm detects the region where the density fluctuations are 2.5 times above the local standard deviation and tracks them in time. If the fluctuations are detected as coherent, they are identified as a blob. The density perturbation associated with each blob is then fitted with a gaussian function that has full width at half maximum, a_{Ri} and a_{Zi} , in the radial and vertical direction (i is the blob index), amplitude n_{bi} and radial velocity

3.3 Investigation of the mechanisms behind the density shoulder formation

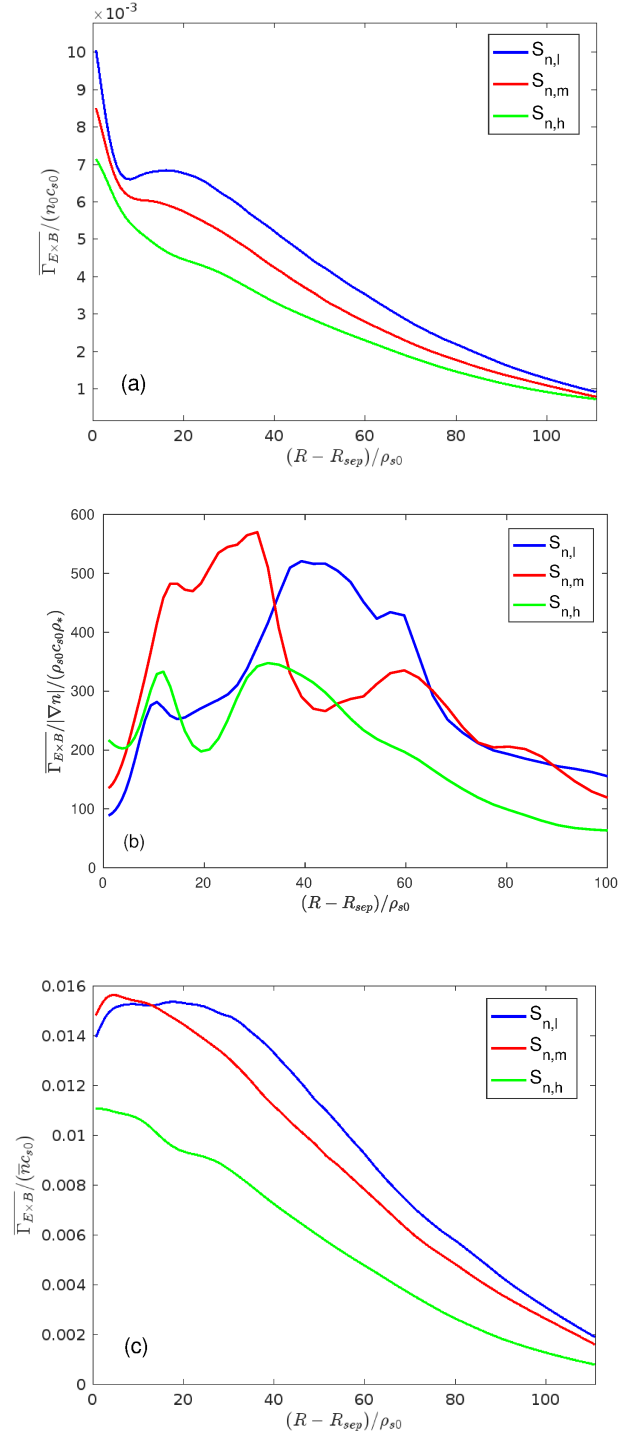


Figure 3.5: Radial profile of perpendicular transport $\bar{\Gamma}_{E \times B}$ (a), $\bar{\Gamma}_{E \times B} / |\nabla n|$ (b) and $\bar{\Gamma}_{E \times B} / n$ (b) at the OMP. All profiles are normalized to their reference value.

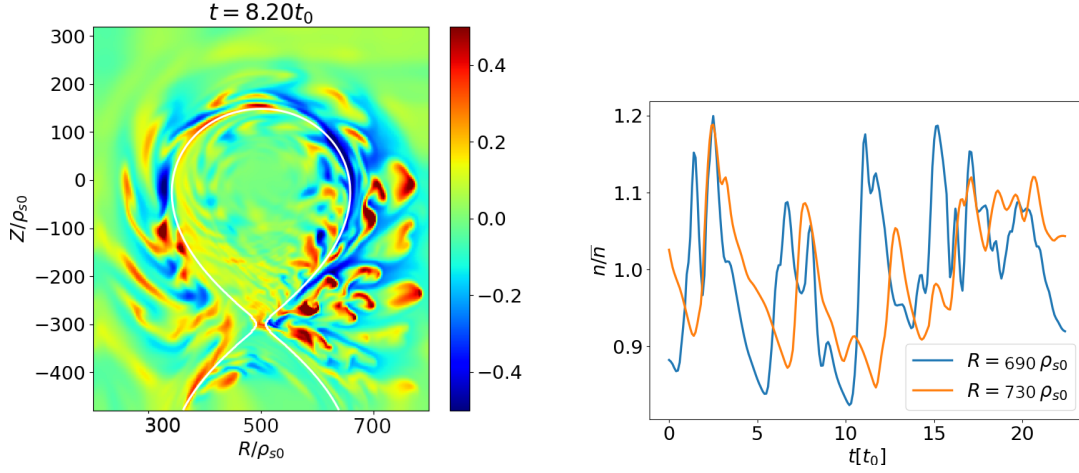


Figure 3.6: Normalized density fluctuations on a poloidal plane (left) and time trace of the density normalized to its average value, for a point in the near SOL, at $(R, Z) = (190, -80)\rho_{s0}$, and a point in the far SOL, at $(R, Z) = (250, -80)\rho_{s0}$.

v_{bi} . The radial transport due to the blobs is then evaluated as the sum of the contribution of all blobs

$$\Gamma_b(R, Z) = \sum_i n_{bi} v_{bi} \exp \left[\frac{(R - R_i)^2}{2a_{Ri}^2} + \frac{(Z - Z_i)^2}{2a_{Zi}^2} \right] \quad (3.2)$$

where (R_i, Z_i) are the coordinates of the center of mass of the i -th blob. From the blobs center of mass motion it is also possible to retrieve the average blob velocities in the poloidal plane, $v_{b,\psi}(R, Z)$ and $v_{b,\chi}(R, Z)$. Our analysis considers all the blobs tracked in the low-field side above the X-point, ensuring statistical convergence to proceed with the detailed study of the $\Gamma_{E \times B}$ flux.

In our simulations, blob transport contribute to about half of the transport in the far SOL [96]. In addition, similarly to [84], blobs are in the RX or RB regimes (i.e., the charge separation inside the fluctuation is damped by parallel resistivity or by the ion polarization current due to the fanning of the flux surfaces [97, 98]), with good agreement between the blob velocity measured in the simulations and the analytical scaling. Thus, we find that the results of the blob tracking analysis are in agreement with the results of previous investigations where the neutral dynamics was not considered.

The histograms for blob size and radial velocity, resulting from the blob tracking algorithm, are shown in Fig. 3.7 separating the near and far SOL. The size is evaluated as the arithmetic average between the radial and poloidal width, which are similar in most cases [99, 97], and the radial velocity as the time-averaged velocity of a blob while the blob is in the region of interest. We first observe that the average blob size increases with S_n both in near and far SOL, leading to a small increase of the average packing fraction from 4% to 4.6%. This is due to a strong decrease of the number of small size blobs, and an increase of the number of larger blobs. The increase of blob size for increasing resistivity is a result well known from previous simulations [99], thus hinting that the effect provided by the addition of neutrals is linked to the change in plasma resistivity. On the other hand, our simulations point out a decrease of the blob velocity with S_n in the far SOL, due to an increase in the number of slow blobs. We note that ionization

processes reduces the electron temperature at high S_n . As we discuss in Sec. 3.3.3 the reduction of the plasma and the blob temperature lowers the radial blob velocity as a consequence of the reduction of the interchange drive [97]. This conclusion is supported by the analysis of the set of simulations with the same power source S_P and density source $S_{n,l}$, $S_{n,m}$ and $S_{n,h}$, that do not include the interaction with neutrals. In fact in simulations without neutrals both the radial velocity and the size of the blobs are observed to increase with ν [82, 99, 97], supporting the idea that the velocity decrease observed with neutrals is indeed due to the presence of neutral interactions. We note that the effect of neutral interactions on blob velocity is discussed in [74], showing a decrease in radial velocity when compared to results without neutrals and with an increase in background density, in agreement with our result.

Experimental evidence hints toward a correlation between blob size and density decay length, which is observed to increase with the edge Greenwald fraction, i.e. the edge density normalized to Greenwald density [78]. In our simulations, the increase in L_n^{near} is in fact correlated with the increase of the blob size, showing a promising agreement with experiments. However, in our simulations larger structures do not correspond to higher turbulent fluxes in the far SOL, as it was hypothesized [76], due to the decrease of the blob velocity. Simulations presented in the next Ch. 4 show that the introduction of molecular deuterium leads to a different OMP radial electric field in the far SOL and higher turbulent fluxes. Experimentally, the relation between blobs radial velocity and edge density was investigated in several devices, but with no conclusive results, showing for example weak proportionality in AUG [88, 100] or inverse proportionality in TCV [41, 78, 101]. The results of our simulations agree with experimental observations, although a detailed comparison should be made to reduce the differences between simulation and experimental setup (e.g., considering a realistic magnetic configuration).

To conclude, our simulations show a decrease of $\Gamma_{E \times B}$ with S_n in the far SOL, due to a reduced blob velocity, despite the larger size of the blobs. As a consequence, the formation of the density shoulder observed in our simulations is not related to an increase of the perpendicular turbulent transport, as proposed from the interpretation of experimental results [76]. Our result is also different from other modelling studies [79], where the density shoulder is obtained through an increase of radial transport, without changes in the ratio $\Gamma_{\perp}/\Gamma_{\parallel}$. In fact, as we show in the analysis of the parallel transport terms, larger S_n is responsible for the reduction of both parallel losses and perpendicular transport. However parallel flux is significantly more affected than the perpendicular transport, increasing the ratio $\Gamma_{\perp}/\Gamma_{\parallel}$. Ultimately, in our simulations the decrease of parallel flux affects plasma density profile more than the changes in the perpendicular flux.

Density decay length estimates

The relationship between decay lengths and perpendicular transport, both in near and far SOL, has been subject of previous investigations in similar configurations without neutrals, where it was developed an analytical estimate for the two decay lengths in this turbulent regime [84].

The estimate for the near SOL density decay length is found balancing the perpendicular heat flux crossing the separatrix with the integral of the heat source over the volume inside it. The first of the two quantities can be estimated as the fluctuating turbulent heat flux associated with the leading order of the perpendicular transport, similarly to what we did for the density flux, $q_{\psi} \simeq \tilde{p}_e \partial_{\chi} \tilde{\phi}$. Linearizing Eqs. (2.88-2.92), the quantity $\partial_{\chi} \tilde{\phi}$ can be expressed in terms of $\partial_t p_e$ and, imposing the saturation of the ballooning instability as the one driving transport, q_{ψ} can be expressed as a function of the pressure decay length L_p^{near} . The perpendicular transport crossing the separatrix can be estimated approximately by

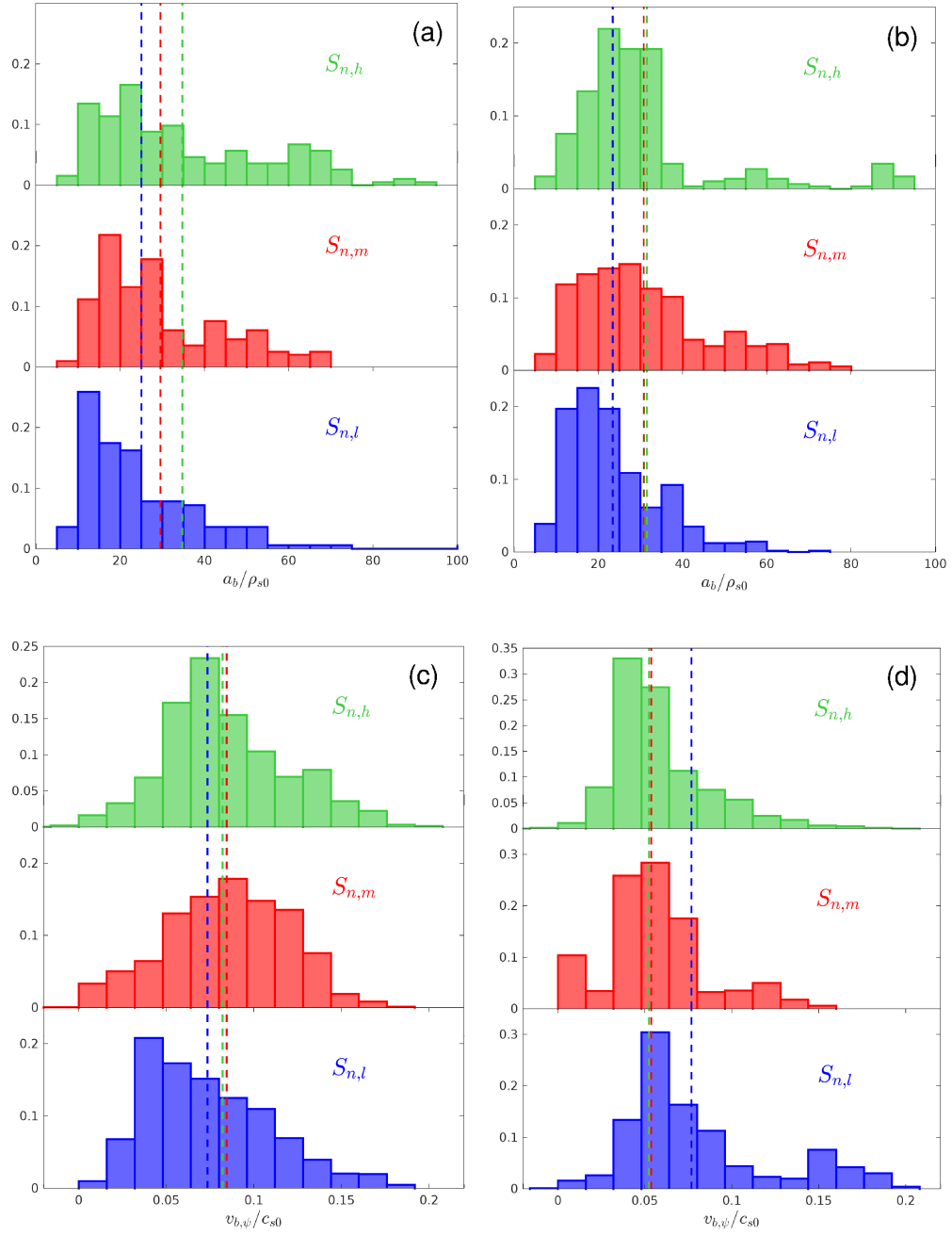


Figure 3.7: Histograms of the blob size for the simulations listed in table 3.1 for near SOL, $R_i - R_{\text{sep}} \in [0, 20]\rho_{s0}$ (a) and far SOL, $R_i - R_{\text{sep}} > 20\rho_{s0}$ (b) and histograms of blob center of mass radial velocity for near (c) and far (d) SOL. The dashed line represents the average value for each quantity and the color is representative of the considered simulation.

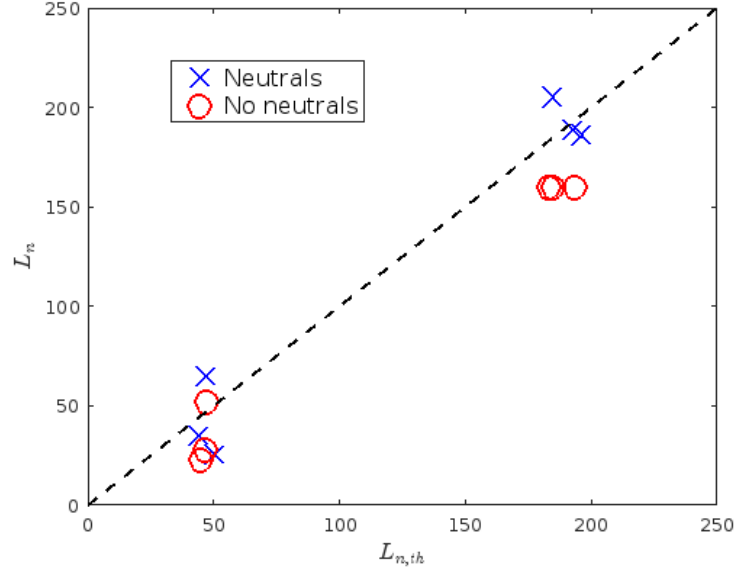


Figure 3.8: Density decay lengths estimated $L_{n,th}$ against measured L_n , for the two set of simulations, with neutrals (blue crosses) and without neutrals (red circles). The cluster of points at lower values identify L_n^{near} , the other cluster is relative to L_n^{far} .

the heat source integrate over the core volume $S_p \simeq \oint_{LCFS} q_\psi dl$, leading to an equation for L_p as a function of the heat source. In this work, we report the estimate for the density decay length, obtained with $L_n \simeq (1 + \eta_e)L_p$ [84], with $\eta_e \simeq 0.77$ [47]

$$L_n = (1 + \eta_e) \left[\frac{1}{8} \left(1 + \frac{\eta_e}{2(1 + \eta_e)} \right)^8 \rho_*^3 \frac{\nu_0^6 q^{12} L_X^{12}}{S_p^4 \bar{n}^{10}} \right]^{1/17}. \quad (3.3)$$

The estimate for the far SOL density decay length can be obtained by balancing the leading order terms in the time evolution of the density equation, Eq. (2.88), in steady state. It can be found that L_n^{far} is proportional to the turbulent flux, i.e. the blob's flux in equation (3.2), leading to

$$L_n^{far} \simeq \rho_*^{-1} \bar{\Gamma}_b \frac{L_\parallel}{\bar{n} \bar{c}_s}, \quad (3.4)$$

with $L_\parallel$ the parallel connection length, $\bar{n}$ the average density and $\bar{c}_s$ the average parallel velocity, equal to the ion sound speed $c_s = \sqrt{T_e/m_{D+}}$.

In Fig. 3.8 the measured decay lengths compared with the estimated ones, showing good agreement between the two, for simulations with and without neutrals interactions. This result suggests that the presence of neutrals do not affect the validity of the estimate L_n^{near} , $L_{p_e}^{near}$, L_n^{far} and $L_{p_e}^{far}$ and therefore the underlying transport mechanisms, but they rather modify the separatrix values of plasma temperature and density.

3.3.2 Parallel transport

Parallel transport appears on the right-hand side of Eq. (2.88) as the divergence of the parallel density flux $\Gamma_{\parallel} = nv_{\parallel e}$. In contrast to the perpendicular transport, fluctuations are subdominant in determining the parallel transport, which can therefore be estimated as $\bar{\Gamma}_{\parallel} \simeq \bar{n} \bar{v}_e$.

In Fig. 3.9 we show $\bar{\Gamma}_{\parallel}/\bar{n}$ along two magnetic field lines located at two different radial distances from the LCFS, indicative of the behaviour in the near and far SOL. The χ coordinate along the magnetic field line is normalised so that $\chi = 0$ represents the high-field side strike point and $\chi = 1$ the low-field side one, whereas the OMP is around $\chi \simeq 0.65$. The dashed vertical lines indicate the χ coordinate at the height of the X-point.

We start our analysis from the near SOL. In the divertor region, the modulus of the plasma velocity increases toward the targets where it reaches the local sound speed, $c_s = \sqrt{T_e/m_i}$. As shown in Sec. 3.3.3, ionization processes lower the electron temperature at large S_n , reducing the parallel velocity at the strike points. However, parallel transport is in general small in the upstream region near the separatrix ($0.2 < \chi < 0.8$), with the presence of two stagnation points that are not significantly affected by S_n . In contrast to the near SOL, a strong difference is observed in the parallel flux at the OMP, $\chi \in [0.65, 0.75]$ in the far SOL. In fact, the parallel flow decreases from the lower to the higher S_n simulation by, approximately, 50%. This results from a decrease of the particle velocity at the inner target in the far SOL, while there is no significant variations at the outer target throughout the simulation scan considered here.

We can then conclude that at large value of S_n , a low parallel transport is observed at the OMP in the far SOL. Interestingly this decrease of parallel transport occurs at the radial distance $R - R_{\text{sep}} > 20\rho_{s0}$, which corresponds to the location where, as shown in Fig. 3.4, we observe the increase of plasma density. This is a result already observed in L-mode experiments, revealing that the Mach number is lower in discharges with higher divertor collisionality [80].

The same analysis carried out for simulations without neutrals supports these results, showing that parallel transport decreases with increasing density source in the core, because higher density source and same input power leads to lower temperature and, consequently, to lower velocities. However, the decrease is stronger when accounting for neutral interactions, where the ionization reactions act as a sink of T_e also in the SOL, further reducing the parallel velocity and the parallel losses.

The analysis of perpendicular and parallel flux gives the possibility to describe the flattening of density profile in terms of the increasing ratio $\Gamma_{\perp}/\Gamma_{\parallel}$. In the near SOL this ratio is approximately independent of S_n , $\Gamma_{\perp}/\Gamma_{\parallel} = 0.021 \pm 0.002$ while, in the far SOL, it increases from a value of $\Gamma_{\perp}/\Gamma_{\parallel} = 0.029$, for the lowest S_n , to $\Gamma_{\perp}/\Gamma_{\parallel} = 0.043$, for the highest S_n . This result confirms that the ratio $\Gamma_{\perp}/\Gamma_{\parallel}$ is important in the shoulder formation, as suggested in [80, 90, 91]. In addition, our analysis shows that this is mostly due to the decrease of parallel transport in the far SOL due to the electron cooling observed at highest values of S_n .

3.3.3 Ionization and interaction with neutrals

Neutral interactions enter directly on the right-hand side of Eq. (2.88) through the ionization source term, proportional to the neutral density and to the ionization frequency. With the increase of S_n , one observes an increase of the ionization rate in the SOL region (see Fig. 3.10). However, the comparison of the local ionization term with the other terms in

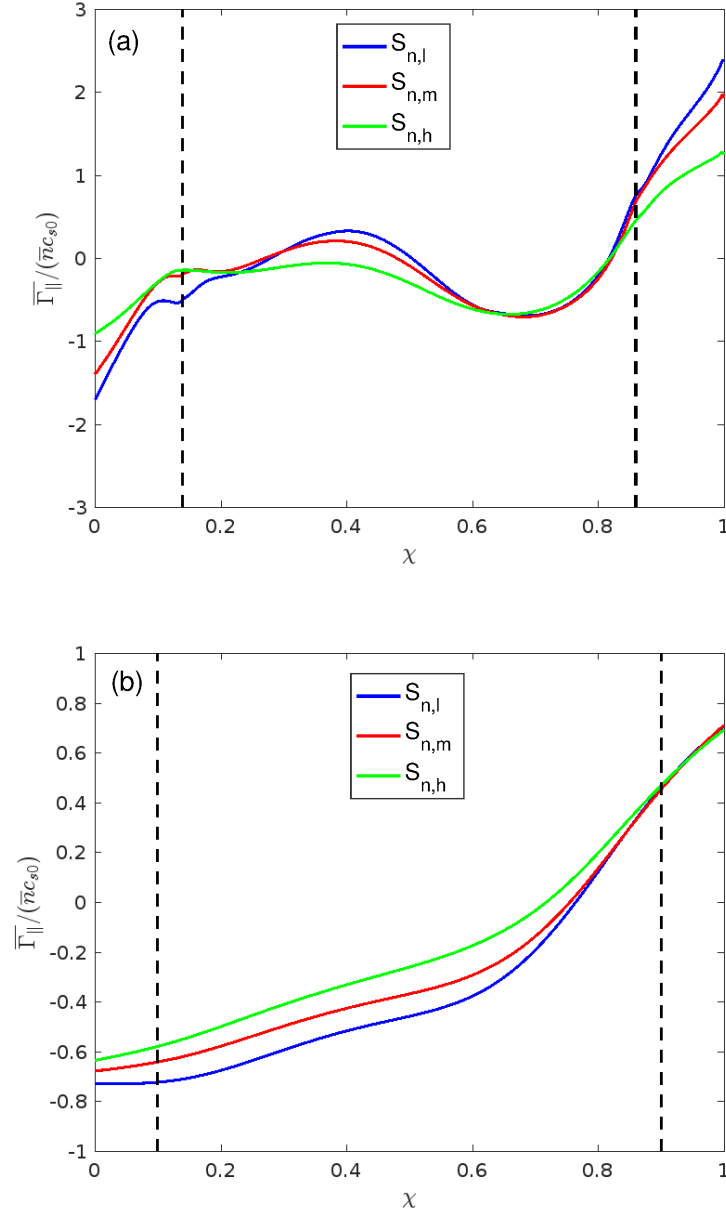


Figure 3.9: Averaged parallel transport profiles along $\nabla\chi$ in a flux tube of width $= 7\rho_{s0}$, in the near SOL, $R - R_{sep} = 4\rho_{s0}$ (a), and in the far SOL, $R - R_{sep} = 70\rho_{s0}$ (b). The black dashed lines indicate the position of the X-point.

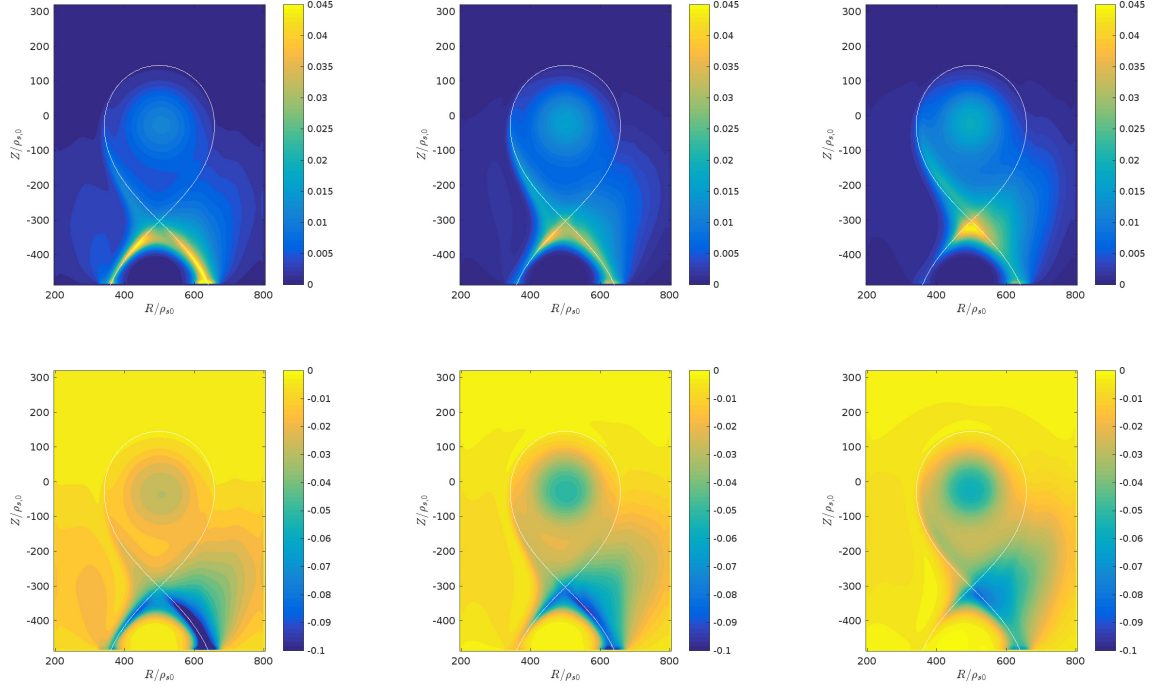


Figure 3.10: Averaged ionization density source, s_n^{neu} (top) and electron temperature neutral interaction term $s_{T_e}^{\text{neu}}$ (bottom), normalized to their reference values. From the left to the right columns the $S_{n,l}$, $S_{n,m}$ and $S_{n,h}$ simulations are considered.

Eq. (2.88) and, in particular, with the divergence of the parallel flux $\nabla_{\parallel} \Gamma_{\parallel}$, shows that the contribution of the local ionization to the density balance at the OMP is negligible. This points out that in our simulations the local source of plasma particle does not play a relevant role in the density shoulder formation, as proposed in other modelling studies [76, 79]. On the other hand, ionization events play a role in the increase of the far SOL density by reducing parallel losses.

We first note that the localization of the ionization source depends on S_n , as shown in Fig. 3.10. At the lowest S_n , the ionization front is localized along the divertor leg, where the density source and temperature sink are most important (see the left column in Fig. 3.10). As S_n increases, ionization events become more important at the X-point, at the OMP and in the core (see the right column in Fig. 3.10). The low temperature reached below the X-point explains the shift of the ionization front towards the midplane with increasing S_n . Figure 3.11 shows the average s_n^{neu} and T_e in the SOL, as a function of the coordinate parallel to the magnetic field χ . We note a decrease of the ionization density source for $T_e < 8\text{eV}$, a threshold below which the ionization rate decreases rapidly, as shown in Fig. 2.1. In addition, the integral of the temperature sink due to ionization reactions in the core, $S_{T_e}^{\text{neu}}$, increases (in absolute value) with S_n , and the temperature sink of the $S_{n,h}$ simulation is larger than the one of the $S_{n,l}$ simulation by 50%. Despite the fact that the amplitude of the temperature source, s_{T_0} , is adjusted to have the same S_P in all the simulations (see table 3.1), the increase of ionization reactions above the X-point is responsible for a reduction of T_e in all the SOL region with the increase of S_n .

Our results are in agreement with recent experimental observations that hint to the importance of high neutral density in

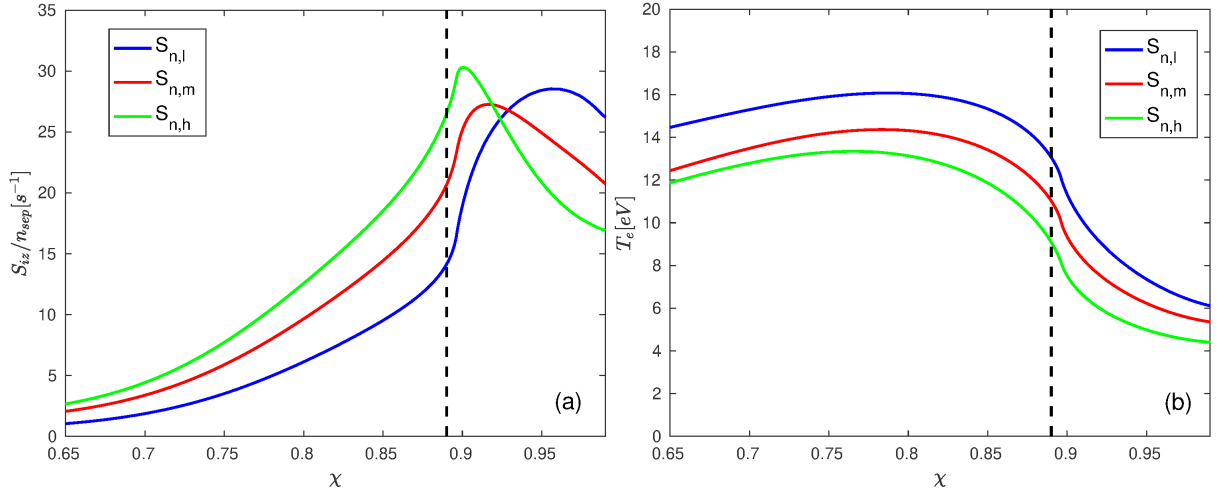


Figure 3.11: Averaged ionization source (a) and temperature profile outside the LCFS (b), in physical units (for an easier evaluation of the cross sections). Quantities are averaged in time, along the toroidal direction and in the radial direction throughout the SOL. The poloidal coordinate is normalized so that $\chi = 0$ at the left strike point, and $\chi = 1$ at the right strike point. In black dashed line the coordinate of the X-point.

the main chamber of tokamaks as a necessary condition to observe the density shoulder [102]. In fact all neutrals emitted near the target can reach the plasma volume in our system, similarly to an open divertor configuration. Therefore, the increased fuelling corresponds to an increase of ionization reactions above the X-point, both inside and outside the LCFS. The increase of S_n reduces the plasma temperature, in the core and SOL region. The lower temperature leads to a reduced parallel velocity, which is ultimately responsible of the density shoulder formation.

3.4 Conclusions

In this chapter we present the first self-consistent GBS simulations of the plasma turbulence and single-species kinetic neutral dynamics in a diverted configuration. We leverage the new capability of GBS to simulate the interplay between plasma and neutrals in arbitrary magnetic configurations and run simulations in steady state with a self-consistent treatment of the particle source as they result from the interaction with the neutrals.

We present results obtained from three different simulations at different core fuelling. The simulations are carried out with a relatively simple model for the interaction of the plasma with the neutrals that includes only ionization, elastic collisions, recombination and charge exchange. However, despite this simplicity, our simulations are able to retrieve some of the most important features associated with the increase of neutral density. For example, an increase in neutral density in the divertor region corresponds to a shift of the ionization peak from the bottom wall to the X-point, as shown in Fig. 3.10. The position of this peak is set by the balance between the drop of T_e due to ionization reactions and the increase of the ionization cross section with T_e .

We observe that the increase in fuelling source causes a reduction of electron temperature, higher resistivity at the LCFS and higher densities in the far SOL. By considering particle balance in the SOL we observe that within the simulated scenarios the higher density is ultimately caused by a reduction of parallel flux due to the lower temperature at the target.

Changes in the ionization and perpendicular fluxes have a lower impact on the OMP density, the first one increasing with increasing density, the second one decreasing. Leveraging methods developed in past studies [84, 99, 89], we perform a detailed investigation of the filamentary transport in the far SOL. When neutral interactions are considered, we observe an increase of the blob-size at higher density source and resistivity, whereas the average blob radial velocity decreases in the far SOL. These results are compatible with recent 2D blob-simulations [74] which showed a slowing down of the center of mass velocity at increased background plasma and neutral density. The mechanisms described by our simulations, where density shoulder is the consequence of reduced parallel transport, seems different from the one observed through diffusive transport models, with density shoulder being obtained by an increase of the perpendicular diffusion coefficient and both perpendicular and parallel fluxes grow [79].

The simulations exhibit the same variation of the near-SOL e-folding length with collisionality that is observed in simulations without neutrals. Such an estimate is compatible with the interpretation suggested in [82] assuming a weak effect of the $E \times B$ shear. On the other hand, it is worth noting that the presence of neutrals could profoundly change the radial electric field pattern [65, 103, 104] at the separatrix and this is a subject further explored in chapter 4. The far SOL scale lengths are observed to be weakly affected by the density source intensity.

Compared with experimental observations, several qualitative similarities may be drawn. As in the experiments, whenever fuelling S_n is increased, our simulations are able to reproduce the increased e-folding length in the near SOL as well as the increase of the blob size. Nevertheless through a detailed analysis of the different transport contributions we are able to associate the increased SOL density to a reduction of the parallel flux, caused by a drop of the temperature because of the increased neutral interactions. The drop in parallel flux is a result seen in experiments [80, 102], but its importance in the density shoulder formation is still under debate [77].

The present analysis constitute a first step in the study of the density shoulder formation with simulations that couple plasma turbulence and the self-consistent kinetic neutral dynamics. In the next chapter, we present the first diverted simulation that include molecular reactions, which play an important role when approaching detached divertor condition.

4 High density turbulent simulations

The second analysis proposed with the GBS model presented in Ch. 2 is the study of turbulence properties in a deuterium plasma with increasing fuelling, trying to understand the influence of molecules in detachment. The work was carried out with the full implementation of the model, running the first GBS simulations of a plasma composed by atomic and molecular deuterium in a diverted configuration. The main results discussed in this chapter are described in an article currently under review.

4.1 Introduction

In order to ensure enough margin towards material fatigue, future devices will need to operate in regimes where a large fraction of the power is dissipated via radiation, ensuring a large pressure drop from the outer mid-plane towards the divertor targets in the unconfined Scrape Off Layer region (SOL) [15, 14, 105]. This can be achieved when tokamaks are operated in detached divertor regime, where core density is increased and a reduction of target temperature, heat and particle fluxes are observed [12, 106, 15]. These losses are largely determined by the plasma-neutral interactions present at low temperatures, $T \lesssim 5$ eV, with an important role played by molecules as sink of particle, momentum and energy [12, 16, 107]. Indeed, neutral atoms and molecules can be ionized at these temperatures, generating atomic and molecular ions at the cost of the ionisation energy, or participate in recombination and charge-exchange reactions, which act as a particle and momentum sink. Molecules can also undergo dissociative processes, increasing the channels for ionization and recombination, e.g. through molecular activated recombination (MAR) reactions. In fact, experimental results show the importance of molecules in detachment. For instance, the role of MAR as ion sink is shown to be dominant compared to the atomic ion recombination [108, 25, 107], producing excited atoms that contributes to the total radiative losses [40, 45], even if the overall importance of these reactions in high density discharges is still debated [109]. The emission of molecules is also influenced by the composition of PFCs. A carbon wall presents a higher probability of recombination on the wall surface, compared to a metal wall where ions are more easily reflected as atoms, with higher energy [40]. Moreover, molecular interactions contribute to momentum losses and they could play an important role in transport balance, helping to understand the asymmetries observed between inner and outer divertor targets [110, 111] and the dependence of the detachment threshold by divertor legs length [15].

A multi-component tokamak plasma is usually described by fluid-diffusive models, for example implemented in SOLPS-ITER [25, 44], or by using fluid and gyrofluid models to reproduce plasma turbulence, for example in SOLEDGE3X (combination of SOLEDGE2D and TOKAM3X) [29] or in GBS [46]. In this work, we present the first multi-component diverted turbulence simulations of a deuterium plasma. The plasma is composed of electrons and two ion species, D^+ and D_2^+ , coupled with a kinetic neutral model that takes into account two deuterium neutral species, D and D_2 . The interplay between molecular interactions, plasma target profiles and turbulent transport is investigated in a lower single null L-mode discharge, with increasing plasma core density. Understanding these processes in L-mode confinement is a first essential step, since it simplifies both the experimental and numerical effort, mitigating the need to understand the transient phenomena induced, e.g. edge localized modes.

The outcome of two different simulations is presented, where the separatrix electron density is increased by a factor of two by increasing D_2 gas puffing introduced at the outer target. With higher density, we find a steady state scenario where the inner strike point (ISP) presents a reduction of ion and heat fluxes, with strong plasma pressure gradient along the magnetic field lines, resembling detached conditions [106]. Our simulations show that molecular interactions affect the plasma dynamics increasing D density in the divertor volume through MAR, modifying the average D temperature and ultimately decreasing the plasma temperature via ionization and charge-exchange reactions. The increase in plasma collisionality due to lower temperature establish strong electric fields in the SOL, with an associated $E \times B$ drift, that increases the plasma asymmetry between the two targets. At the outer mid-plane (OMP) we observe the formation of a density shoulder [68], due to the increase of turbulent transport observed in high resistivity scenarios [68, 95, 78, 112].

The present chapter is organised as follows. After the introduction, in Sec. 4.2 we provide a description of the simulations setup, followed by an overview of the results obtained from the comparison of the two simulations, their average profiles and the analysis of the role of molecules. The analysis of the target and OMP fluxes, including the role of the $E \times B$ drift and the analysis of turbulence, is described in Sec. 3.3. The conclusions follow.

4.2 Overview of the simulations results

In this section we provide a description of the simulations used in this work, providing their configuration and the comparison of their plasma and neutrals profiles. We start detailing the setup of the simulations in Sec. 4.2.1 and showing the density profiles for both plasma and neutrals in Sec. 4.2.2. In Sec. 4.2.3 we discuss the pressure and temperature profiles, together with the analysis of the energy sink due to neutral interactions. To conclude, we present in Sec. 4.2.4 the results on the electric fields observed in our high-density simulations.

4.2.1 Simulations setup

In this work we consider two simulations carried out with the GBS code implementing the model described in Ch. 2. The simulation parameters are based on an experimental dataset developed for validation studies, TCV-X21 [67]. TCV-X21 is a lower single-null L-mode discharge performed at low toroidal magnetic field, with value at magnetic axis $B_0 = 0.9$ T, in forward field direction (ion- ∇B drift direction pointing from the core toward the X-point), with plasma current $I_p=165$ kA. The upstream experimental density and electron temperature at the separatrix, taken as reference density and temperature in the simulations, are $n_0 = 0.6 \times 10^{19} \text{ m}^{-3}$ and $T_{e0} = 35$ eV. This corresponds

to ion sound Larmor radius $\rho_{s0} \simeq 1$ mm, sound speed $c_{s0} \simeq 4.1 \times 10^4$ m/s and reference time $t_0 = 0.02$ ms. Given the explorative nature of the present study, the computational cost of the simulation is reduced by considering a domain corresponding to half the size of the TCV tokamak ($R/a = 0.8/0.25$ m), i.e. $L_R = 300 \rho_{s0}$, $L_Z = 600 \rho_{s0}$ and $L_\varphi = 2\pi R_0 \simeq 2800 \rho_{s0}$. The dimensionless simulation parameters are $\rho_*^{-1} = 450$, $\tau = 1$, $\eta_{0e} = 3 \times 10^{-4}$, $\eta_{0D^+} = \eta_{0D_2^+} = 2 \times 10^{-2}$, $\chi_{||e} = 20$, $\chi_{||D^+} = \chi_{||D_2^+} = 1$, $m_i/m_e = 2500$, $\beta_{e0} = 2 \times 10^{-6}$, and $\nu_0 = 0.05$. The diffusion coefficients are set to $D_f = 15$, for $f = \{n, T_e, T_{D^+}, T_{D_2^+}, \Omega, U_{||e}, v_{||D^+}, v_{||D_2^+}\}$, and are verified to be at least one order of magnitude lower than the other effective transport coefficients evaluated in the transport analysis of our results, $D_{E \times B, \text{eff}}$ in section 3.3. The amplitude of the temperature source is chosen so that the power source, integrated over the core region, corresponds to the experimental estimated value of the power crossing the separatrix in the TCV-X21 case, $P_{\text{sep}} = 120$ kW [67]. These parameters are chosen to mimic the typical conditions found in L-mode diverted discharges, as described in Ref. [66], where turbulent transport is mostly interchange dominated and it is characterized by eddies developing near the separatrix.

Regarding the parameters that describe the neutral-plasma interaction, we consider an effective ionization energy of $E_{iz} = 30.0$ eV, taking into account the radiation losses that occur with ionization [12]. Recycling at the top and right walls, where no strike points are present, is found to be negligible, thus it is not considered. For all four walls a constant reflection coefficient, $\alpha_{\text{refl}} = 0.2$, and an association coefficient $\beta_{\text{ass}} = 0.1$ are considered. The gas puffing is positioned on the bottom wall, with a narrow gaussian profile centered at $R/\rho_{s0} = 150$, corresponding to one of the gas puff positions present in TCV. The neutrals are emitted from the wall and are puffed at room temperature $T_{\text{wall}} = T_{\text{GPD}_2} = 0.03$ eV.

The two simulations presented in this work have the same setup, except for the strength of the D_2 gas puff on the bottom wall. In the first simulation there is no puffing and neutrals come only from plasma recycling and recombination, we label it *low density*. In the second simulation we increase the neutrals and plasma density introducing a gas puff of D_2 , we label it *high density*. We start the low density simulation introducing molecular association and recombination in a quasi-steady state simulation with only atomic neutrals interactions [31]. After approximately $20 t_0$ we find the turbulent quasi-steady state in the low density simulation, where losses at the vessel balance the particle sources. The high density simulation is then obtained introducing the D_2 gas puff in the quasi-steady state of the low density simulation.

Regarding the numerical parameters used in our simulations, we note that we use a grid for the plasma $N_R \times N_Z \times N_\phi = 150 \times 300 \times 64$, while the grid for the neutrals is $N_R^n \times N_Z^n \times N_\phi^n = 50 \times 100 \times 64$. The time step for the plasma evolution is $\Delta t \simeq 3 \times 10^{-5} t_0$, while the solution for the neutral model is evaluated every $\Delta t \simeq 0.1 t_0$. The grid used and the neutrals evaluation frequency ensure that our simulation results are converged [31]. After a transient the simulations reach a quasi-steady state where plasma and neutral quantities oscillate around constant values. The average profiles are evaluated over an interval $\Delta t = 10 t_0$. In the analysis we also present flux tube averages that leverage the magnetic field aligned coordinate system introduced in Ch. 2 and used in Ch. 3, where the poloidal coordinate χ goes from $\chi = 0$ at the ISP to $\chi = 1$ at the OSP and the radial coordinate is expressed as $\rho_\psi = \sqrt{(\psi - \psi_{\text{axis}})/(\psi_{\text{xpt}} - \psi_{\text{axis}})}$, having $\rho_\psi = 1$ at the last closed flux surface.

4.2.2 Plasma and neutrals density profiles

The two simulations allow us to explore the dynamics at two different separatrix densities. The low-density simulation is characterized by $n_{e,\text{sep}} = 1.62 \times 10^{19} \text{m}^{-3}$ and the high density by $n_{e,\text{sep}} = 3.42 \times 10^{19} \text{m}^{-3}$ at $Z = Z_{\text{axis}} = 0$. In Fig. 4.1 and Fig. 4.2 average profiles of the electron and molecular ion densities on the poloidal plane are shown for the low and high density simulations, together with a snapshots of their fluctuations (we will denote with tilde the fluctuating quantities and with the overline their time average, e.g. $n_e = \tilde{n}_e + \bar{n}_e$).

The high density simulation presents not only increased core density, but also increased density in the SOL region, with higher level of turbulence fluctuations. Similar descriptions of the increase of turbulent fluctuation amplitude with density are reported in Ref. [95, 66]. The D_2^+ density is at least two orders of magnitude lower than the electron one and, as a consequence, $n_{\text{D}^+} \simeq n_e$, as assumed by the model. The high density simulation exhibits strong enhancement of the plasma density in the private flux region close to the OSP, not observed at the ISP, resulting from the balance of the fluxes and the colder target existing at higher plasma density, as discussed in Sec. 4.3. The density of molecular ions is large in the region close to the targets, with a negligible value inside the last closed flux surface.

In Fig. 4.3 we show the time averaged profile of the neutral densities n_{D} and n_{D_2} , while in Fig. 4.4 we show the density source of electrons from D and D_2 ionization, together with the recombination density sink. At low density, neutrals are produced through recombination at the wall and recycled at the target, most of the ionizations occurring close to the targets. With the introduction of the gas puff, molecular neutrals penetrate deeper in the tokamak volume and the ionization front enters the edge and core. D_2^+ ions are produced by ionization of D_2 neutrals, therefore their density is directly related to the dynamics of the neutral molecules and the value of the density n_{D_2} . In particular, the $n_{\text{D}_2^+}$ profile is the result of the balance between D_2 ionization, mainly in the divertor volume, and transport toward the targets, explaining high $n_{\text{D}_2^+}$ close to the target regions. Even if the increase of ion density leads also to the increase of recombination reactions, the magnitude of the recombination peak is one order of magnitude lower than the ionization peak, becoming relevant only close to the OSP. The profile of S_{n_e} in a flux tube along the SOL close to the separatrix, for $1 \leq \rho_\psi \leq 1.1$, is presented in figure 4.5, showing that the dominant neutral interactions in eq.(2.39) are characterized by ionization above the X-point and by recombination close to the wall. It's interesting to notice the asymmetry between the ISP and OSP, mainly given by the asymmetry in $n_{\text{D}_2^+}$ and n_{D^+} profiles, that are the result of the balance between D_2 ionization and recombination, and transport toward the targets.

Focusing on the atomic neutrals, we note that the increase of their density in the high-density simulation is a combined effect of the increase of recombination and decrease of the ionization processes they can undergo. In fact, as table 2.1 shows, atomic neutrals are produced through recombination, dissociation of D_2 or D_2^+ and MAR processes. By performing a set of simulations where we artificially remove one of these reactions at a time, we identify MAR reactions as the main source of n_{D} in our high density simulation. Indeed they account for 40% of the neutrals are produced. This result is in agreement with experimental findings, where recombination activated by molecules in high density discharges is estimated to be dominant compared to other recombination channels [25, 107]. The decrease of the number of ionization processes in the target regions, a consequence of the strong decrease of the local temperature to values smaller than 3 eV (see Sec. 4.2.3), leads also to an increase in n_{D} .

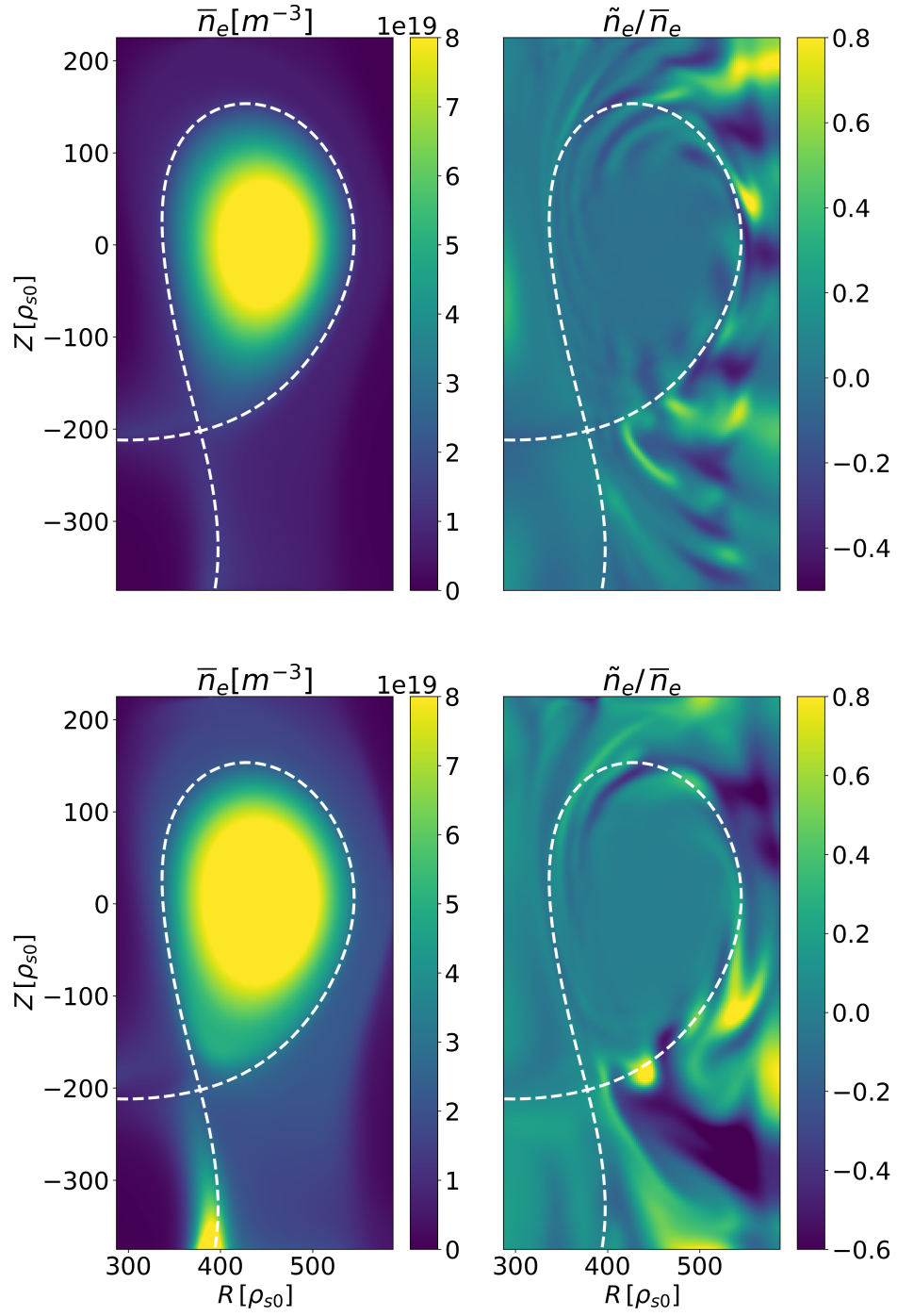


Figure 4.1: Average of the poloidal electron density n_e , with a snapshot of the normalized fluctuations, for the low density (top row) and high density (bottom row) simulations.

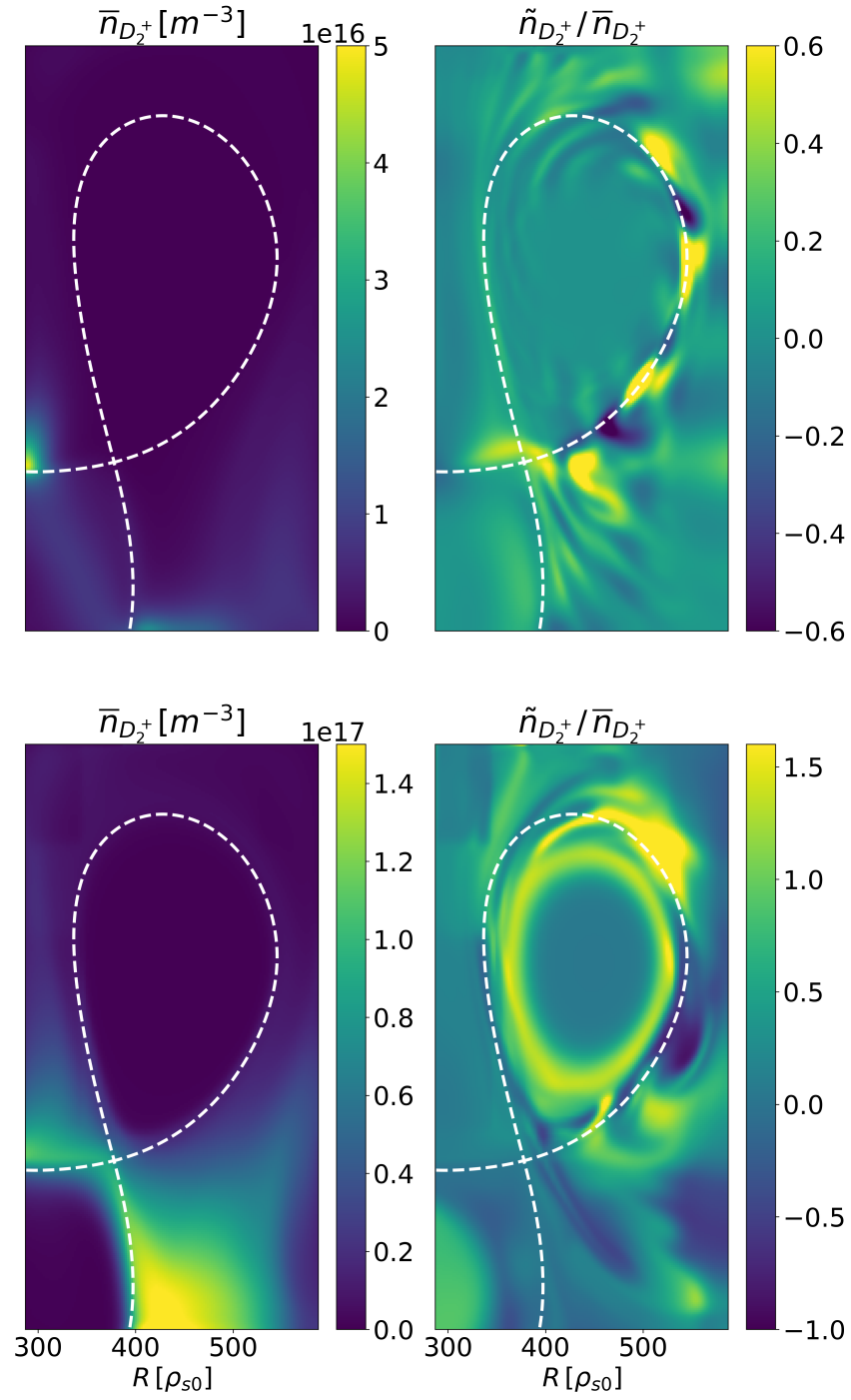


Figure 4.2: Average of the poloidal molecular ion density $n_{D_2^+}$, with a snapshot of the normalized fluctuations, for the low density (top row) and high density (bottom row) simulations.

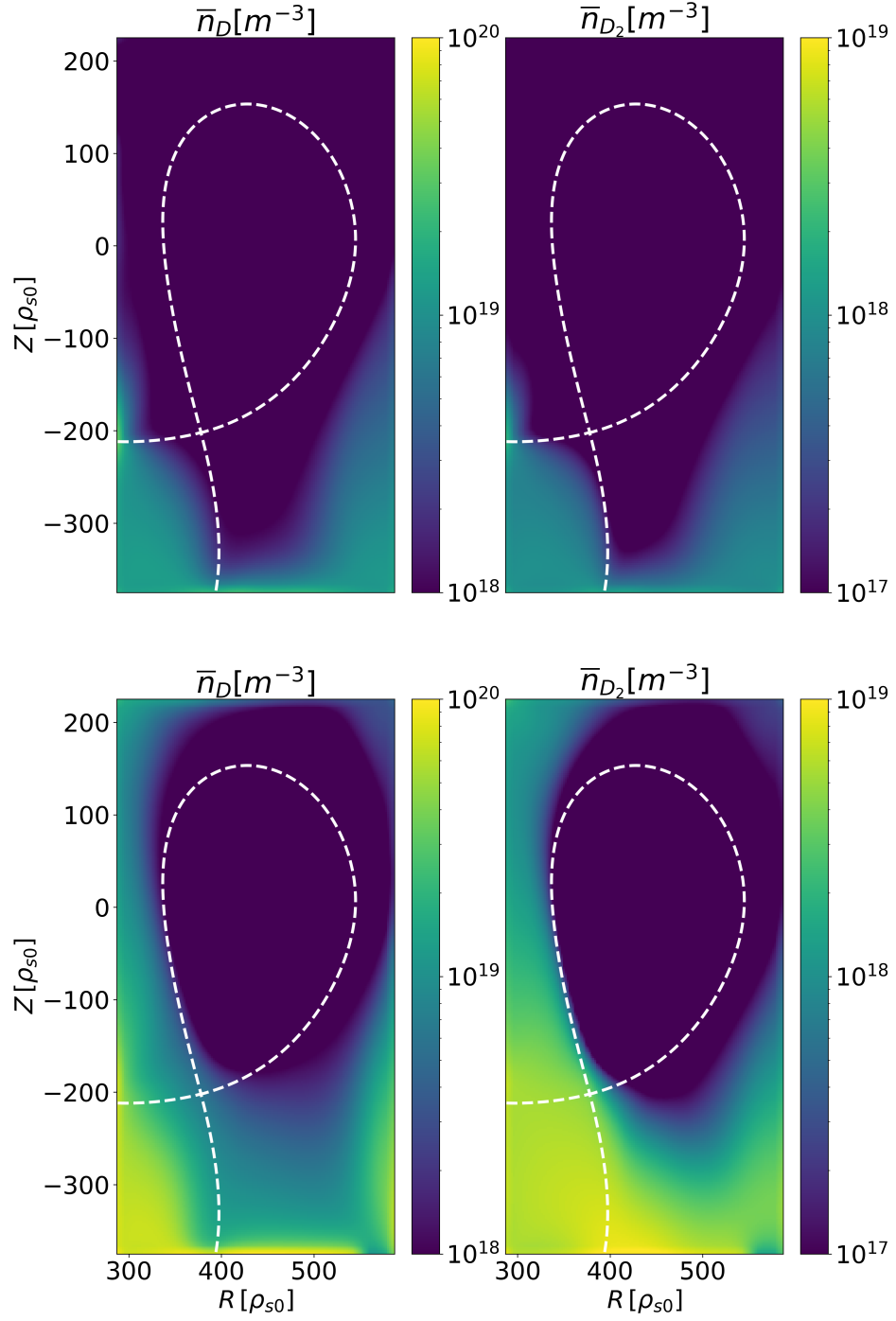


Figure 4.3: Time and toroidal averages of the poloidal atomic neutrals density n_D and molecular neutrals density n_{D_2} for the low density (top row) and high density (bottom row) simulations.

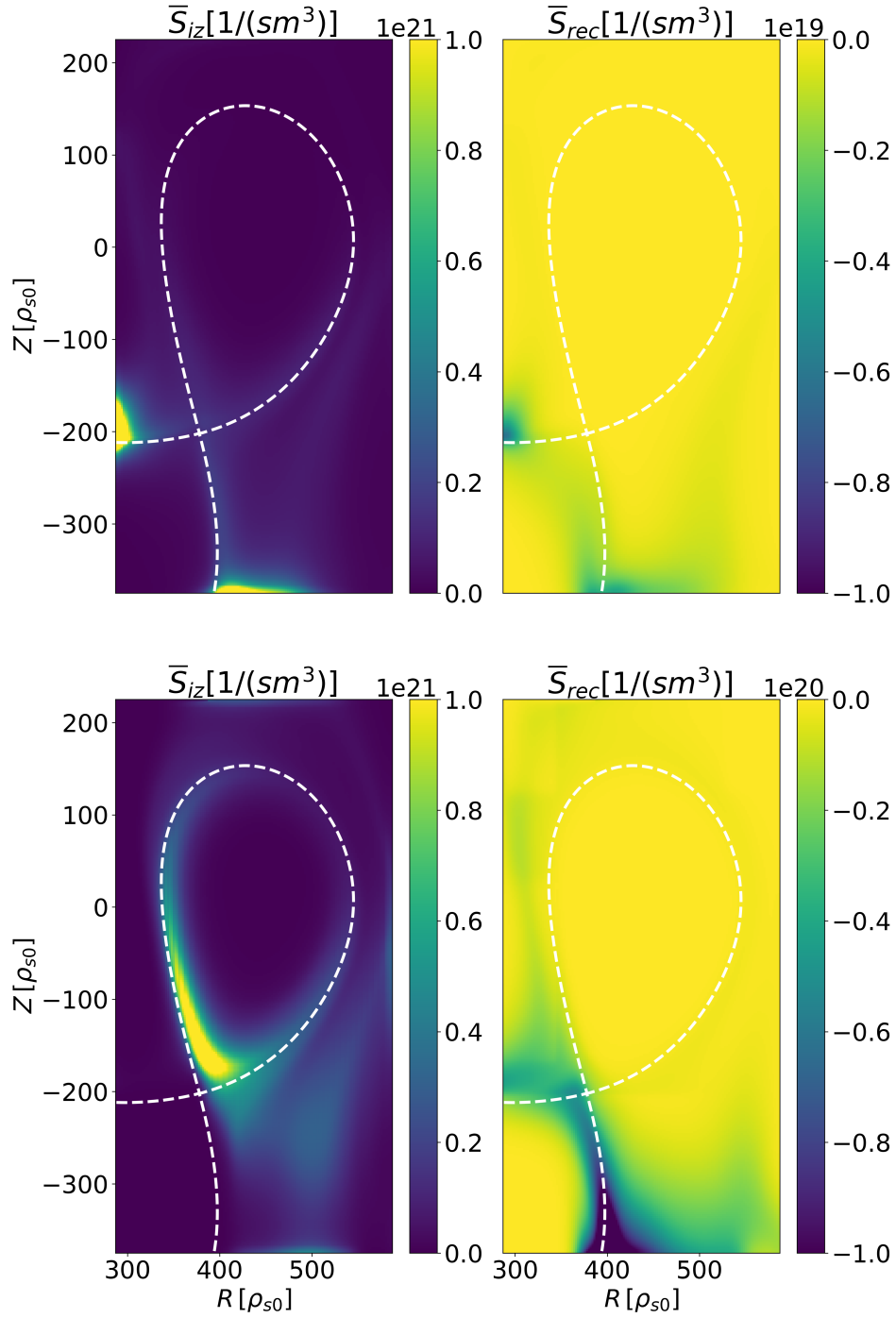


Figure 4.4: Time and toroidal averages of the electron density source due to ionization and electron density sink due to recombination, for the low density (top row) and high density (bottom row) simulations.

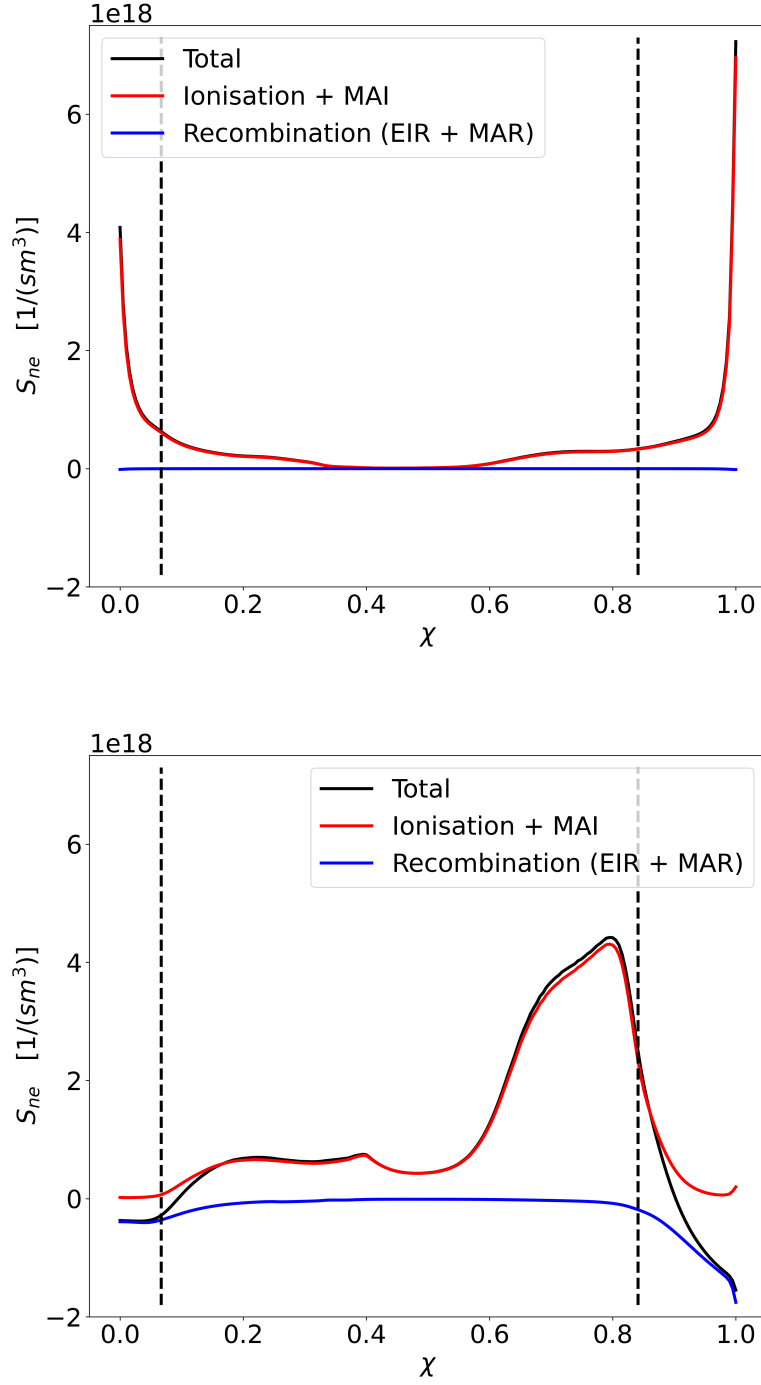


Figure 4.5: Averages of the electron density source and sink due to plasma-neutral interactions for the low density (top) and high density (bottom) simulations, along a flux tube close to the separatrix $1 \leq \rho_\psi \leq 1.1$, as a function of the poloidal coordinate χ . In black dashes the X-point coordinate.

4.2.3 Pressure drop and target temperature

A detached scenario is characterized by very low plasma temperature at the target, $T_e < 3$ eV, with a pressure drop between the upstream (OMP) region and the target [106]. The temperature decrease is often observed simultaneously with the increase of radiative losses due to interaction with neutrals. Radiation is important in the SOL region up to the X-point [15, 111]. The low target heat flux together with high pressure drop is also the result of momentum loss mechanisms, e.g. due to ion-neutral charge-exchange reactions [12, 113].

The energy losses by plasma-neutral interactions in our model are obtained by combining the density and temperature sources Eqs.(2.45-2.47), as shown in Eq. (2.54). The losses associated with the different reactions evaluated separately in order to estimate their relative importance, are shown in Fig. 4.6. In the low density simulation, ionization processes are relevant only in the target regions and the energy loss occurs below the X-point ($\chi_{\text{Xpt, HFS}} = 0.05$, $\chi_{\text{Xpt, LFS}} = 0.86$), where both ionization and charge-exchange losses increase due to the increase of neutral density. On the other hand, the high density simulation presents stronger energy losses in a considerable larger volume, also above the X-point, where the ionization sink presents a peak. We point out that the integral of the energy losses above the X-point in the high density simulation is twenty times higher compared to the low density one, mainly due to the local n_D increase due to molecular interactions [107, 45]. Along the outer divertor leg, for $0.85 < \chi < 0.95$, both atomic and molecular ionizations are practically absent and the main energy sink are is due to radiative losses caused by D_2 and D_2^+ dissociation, except close to the target where charge-exchange becomes the dominant reaction. Along the inner divertor leg, for $\chi < 0.08$, we observe a lower contribution of molecular dissociation, making charge-exchange the main loss mechanism. Higher molecules density increases energy losses along all the flux tube profile, increasing charge-exchange reactions above the X-point, both in HFS and LFS, and increasing the radiative losses along the divertor legs.

Figure 4.7 shows the average total pressure and D^+ ion parallel velocity, along the same flux tube of Fig. 4.6. We evaluate the total pressure as the sum of the static and dynamic pressure of each species:

$$p_{\text{tot}} = n_e T_e + n_{D^+} (T_{D^+} + m_{D^+} v_{D^+}^2) , \quad (4.1)$$

since the contribution of $n_{D_2^+}$ is negligible compared to the others, as well as the electron dynamic pressure.

In both simulations the D^+ fluid presents a stagnation point close to the OMP, $\chi = 0.7$, and its module increases toward the two targets, as observed in previous simulations [68]. However the high density simulation presents lower velocity at both divertor targets, as expected by the larger importance of charge-exchange reactions. Both pressure profiles present a maximum around the OMP, where the density and temperature are higher. In the high density case the pressure is higher at the OMP and lower at the targets, resulting in a larger total pressure drop than the low density case. Comparing Fig. 4.6 and 4.7, it is possible to observe that the peaks of power loss located at $\chi = 0.18$ and $\chi = 0.80$ (see Fig. 4.6) are associated with a strong pressure drop, indicating that plasma-neutral interactions plays a determinant role as pressure sink of our simulations.

The relative importance of the atomic reactions along a flux tube is mainly determined by the plasma temperature profile [37]. The temperature of all the species present in our simulations are shown in Fig. 4.8. In both simulations the temperature of the molecular species are lower than the others, while the D^+ and electron temperatures are very similar. At low density, the plasma temperature decreases because of the ionizations occurring close to the target, causing a steep

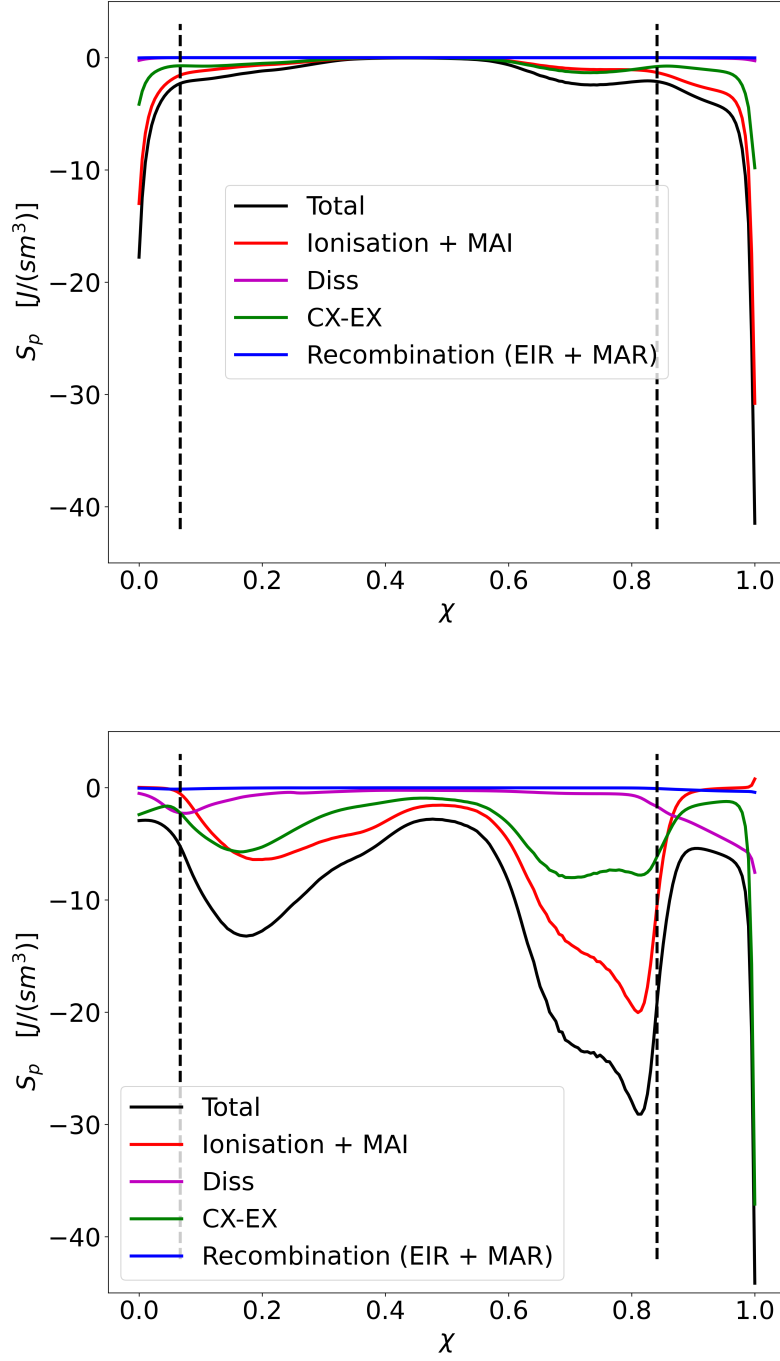


Figure 4.6: Averages of the energy sink due to plasma-neutral interactions for the low density (top) and high density (bottom) simulations, along a flux tube close to the separatrix $1 \leq \rho_\psi \leq 1.1$, as a function of the poloidal coordinate χ . In black dashes the X-point coordinate.

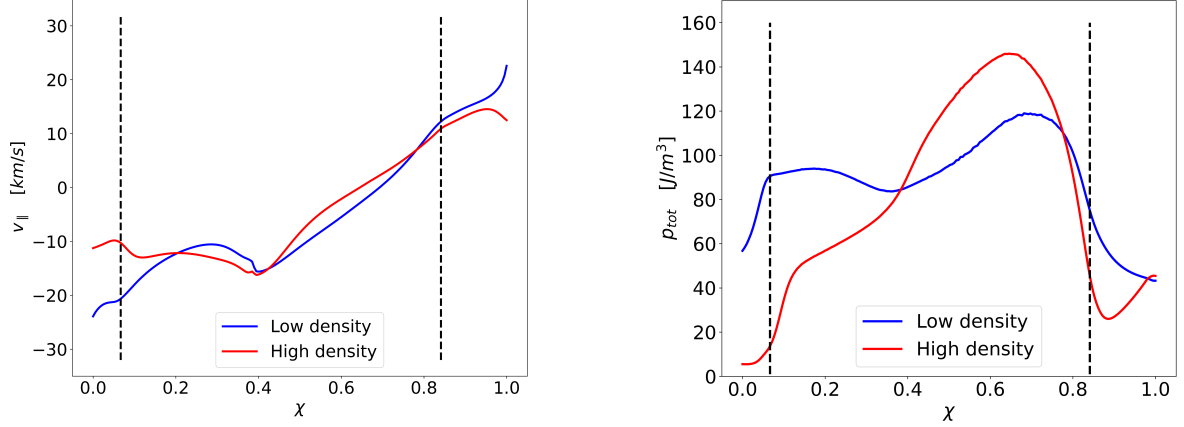


Figure 4.7: Averages of the ion parallel velocity (left) and total plasma pressure (right) along a flux tube close to the separatrix $1 \leq \rho_\psi \leq 1.1$, as a function of the poloidal coordinate χ . In black dashes the X-point coordinate.

temperature gradient in the divertor regions. Since the temperature remains above 3 eV, in this simulation recombination and dissociation reactions are negligible and neutrals are emitted mainly from the wall. A fraction $\alpha_{\text{refl}} = 0.2$ are emitted at the ion temperature (see Ch. 2) and the remaining are released at the wall temperature $T_{\text{wall}} = 0.03$ eV, explaining the value of T_D .

In the high density simulation the temperature of the charged species is sufficiently high to ionize the neutrals ($T_e > 3$ eV) above the X-point, while this is not the case closer to the target, a condition that is denoted as power starvation [114]. Neutrals are produced in the divertor volume through dissociation and recombination processes, at a temperature of 3 eV (see Table 2.2), or at the wall. The resulting temperature at the target is asymmetrical between the ISP and the OSP due to the asymmetries in molecules density profiles, ultimately determined by the gas puff position. The plasma energy loss due to charge-exchange are dominant at the targets (see Fig. 4.6), lowering the plasma temperature. In particular, at the outer target, the presence of the D_2 puff leads to higher D density, resulting in increased charge-exchange processes and ultimately in $T_{D+} \simeq T_D$.

4.2.4 Plasma potential and ohm's law

Strong electric fields in the divertor volume of high-density discharges are predicted and observed experimentally [115, 116], leading to $E \times B$ flows in the poloidal plane [117, 118]. Our simulations confirm the presence of those flows.

The average plasma potential profiles obtained in both simulations are shown in Fig. 4.9. In both cases the potential presents positive values in the SOL, higher in the LFS and around the X-point. A positive plasma potential at the X-point was already observed in simulations and experiments with the same magnetic field direction [115]. In the high-density case the value of ϕ increases in the far SOL, the positive region enlarges in the radial direction, while decreasing close to the targets. The result is the presence of an electric field pointing toward both targets and inside the private flux region in the high-density plasma. This is relevant to explain the transport mechanisms at play in the high density simulation, as described in Sec. 3.3.

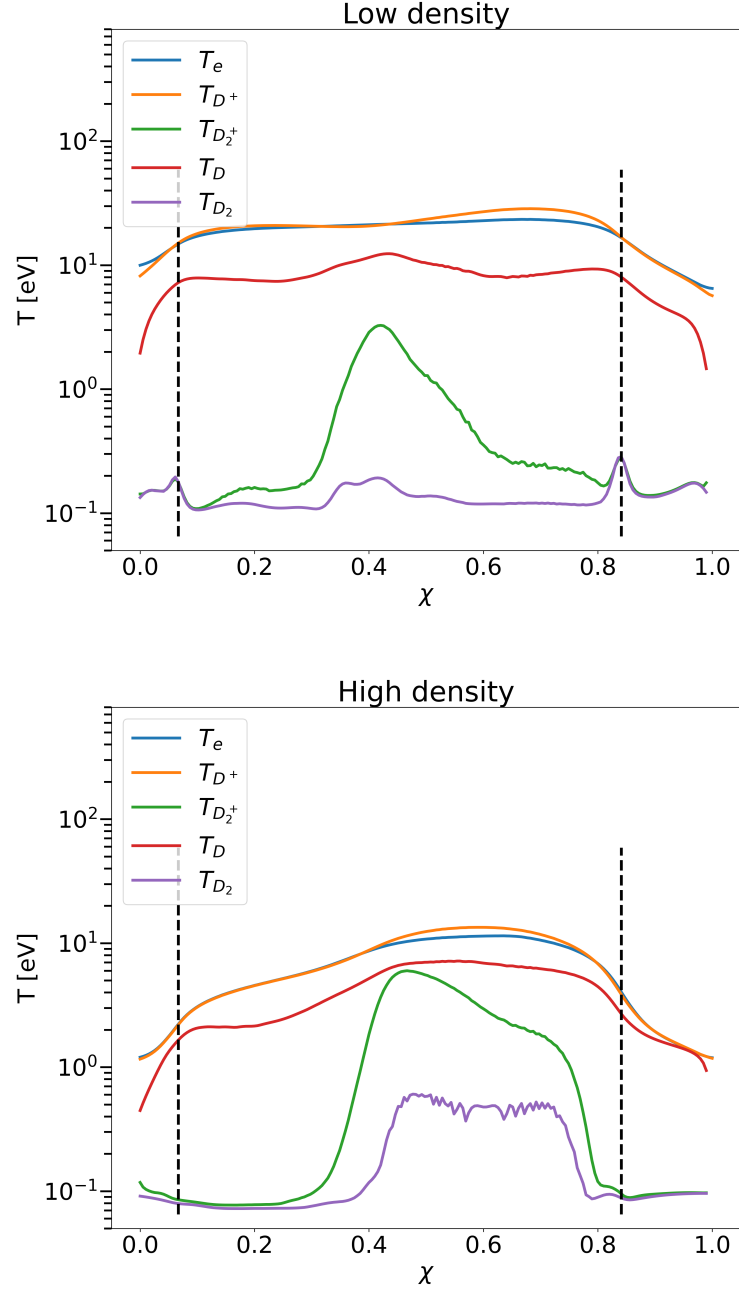


Figure 4.8: Averages of all the species temperatures for the low density (left) and high density (right) simulations, in a flux tube close to the separatrix, $1 \leq \rho_\psi \leq 1.1$, as a function of the poloidal coordinate χ . In black dashes the coordinate of the X-point.

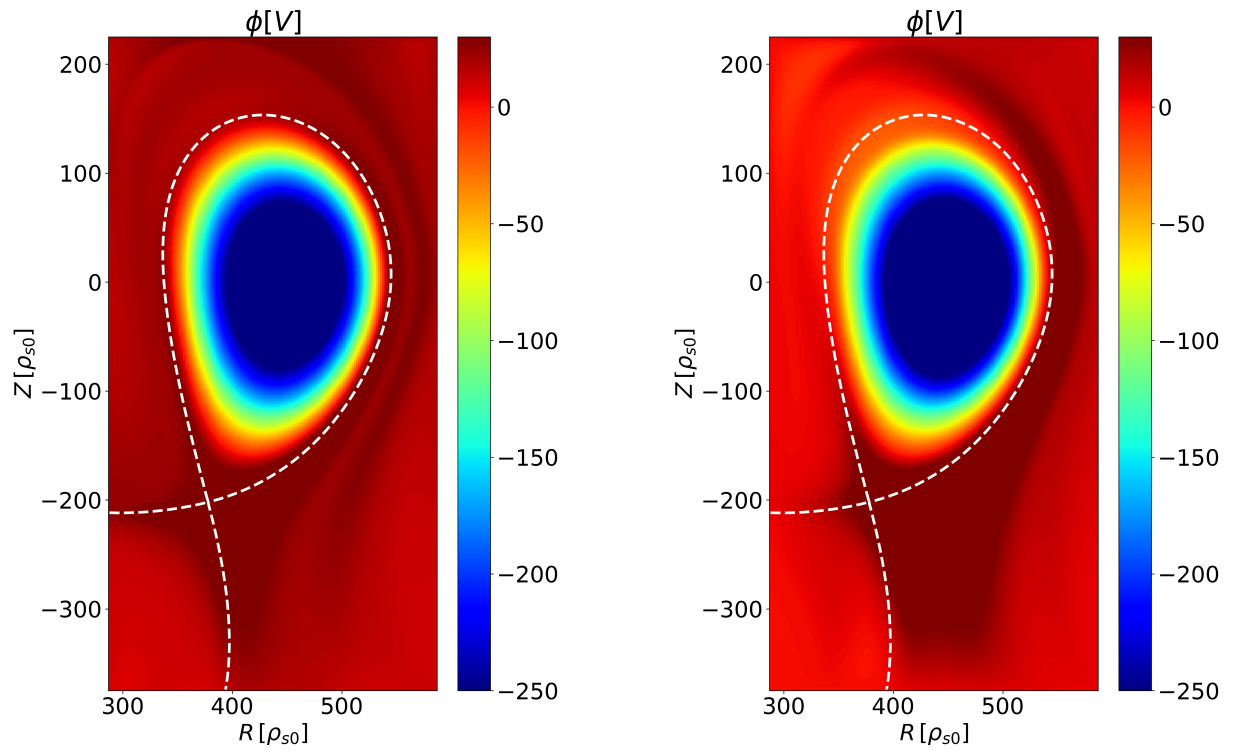


Figure 4.9: Average profiles of the plasma potential of the low density (left) and high density (right) simulations.

The origin of the electric field can be studied by analysing the generalized Ohm's law, Eq.(2.42), that defines the relationship between parallel gradients of potential, electron temperature, pressure and parallel current

$$E_{\parallel} = -\nabla_{\parallel}\phi = \frac{\nabla_{\parallel}p_e}{n_e e} + 0.71 \frac{\nabla_{\parallel}T_e}{e} - \nu j_{\parallel}, \quad (4.2)$$

having neglected electron inertia. In Fig. 4.10 the time-averaged terms appearing in Eq.(4.2) are shown along the radial direction in a flux tube close to the separatrix. For both simulations the parallel electric field follows the profile of the term proportional to plasma resistivity ν , defined in Eq.(2.50). In the high density case the relative importance of this term is increased, especially close to the target where the temperature is lower, being $\nu \propto T_e^{-3/2}$. Experimentally, it is observed that in discharges with relatively high temperature at the target, $T_{e,\text{targ}} \geq 20$ eV, the resistive term do not influence the plasma potential at the OMP [119]. Our results show that collisionality determines the potential along the flux tube, between target and mid-plane, when the plasma temperature is low.

4.3 Transport in high-density plasma

Detachment is characterized by reduced ion and heat fluxes at the divertor targets compared to attached discharges [106]. In the following, we analyse divertor and target fluxes, along with turbulent transport at the OMP.

4.3.1 Ion target flux and particle balance

When a density ramp is experimentally performed, the divertor moves across different recycling conditions, from attached, to high-recycling, partial and finally full detachment conditions [106, 111]. The roll-over of the target ion flux identifies the onset of detachment, i.e., as the plasma density increases, the peak ion flux at the target does not and the reduction of the ion flux integral at the target is observed. The onset of detachment at the ISP and the OSP in lower-single null discharges often occurs at different level of density [110], with the differences between the two legs depending on the field direction, pointing out to a possible role of the $E \times B$ drift [111]. In fact, simulations of the different phases of detachment, carried out with SOLPS-ITER, show that the introduction of drifts improves the comparison with experimental measurements [44].

In Fig. 4.11 we show the particle flux profile in our simulations, in the left wall region that surrounds the ISP and, similarly, a region of the bottom wall around the OSP. The ion flux at the target is evaluated as the sum of the parallel flow and the drifts motion, in the direction perpendicular to the target:

$$\Gamma_{D^+,j} = n_{D^+}(v_{\parallel D^+,j} + v_{\perp D^+,j}) = n_{D^+}(v_{\parallel D^+} b_j + v_{E \times B, D^+,j} + v_{di,j}), \quad (4.3)$$

where b_j is the j component of the unit vector along the direction of the magnetic field, with $j = R$ or Z , for the ISP and OSP respectively.

In figure 4.11 we show the particle flux profile in our simulations, for a section of the left wall that includes the ISP and for a section of the bottom wall that includes the OSP.

Focusing on the low density simulation, the ion flux at the ISP is approximately symmetric around its maximum, which

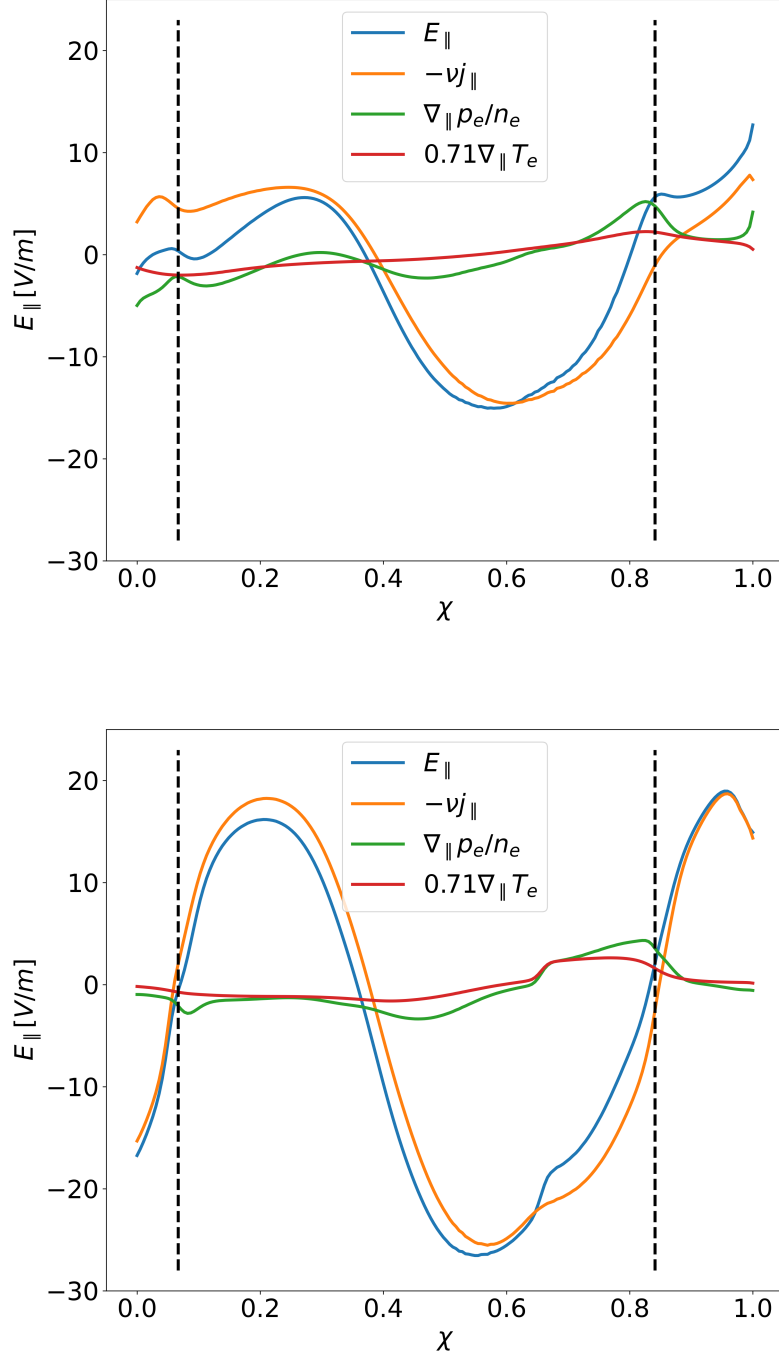


Figure 4.10: Average profile of the parallel electric field and its components according to the generalized Ohm's law, in a flux tube close to the separatrix, $1 \leq \rho_{\psi} \leq 1.1$, as a function of the poloidal coordinate.

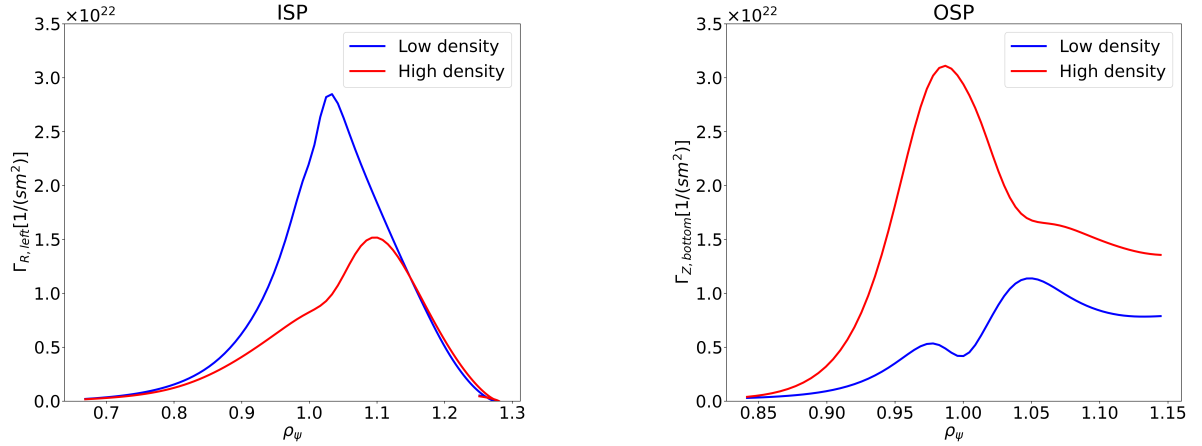


Figure 4.11: Average of the ion particle flux at the target, for both strike points, as a function of the normalized poloidal flux function.

is located in the SOL ($\rho_\psi > 1$). On the other hand it is possible to identify a double peak at the OSP, one in the SOL and a second one in the private flux region ($\rho_\psi < 1$). For both targets the larger contribution is given by the parallel flux, responsible for the peak in the SOL, while the $E \times B$ flux is dominant for $\rho_\psi < 1$, transporting density from the ISP to the OSP. This is consistent with SOLPS simulations showing that the inclusion of $E \times B$ drift in the plasma dynamics can lead to the formation of a double peak in the target profiles, together with higher density at the ISP or at the OSP for, respectively, forward or reversed field configuration [120, 121].

The density increase affects the ion flux differently at the two targets. At the ISP the integral of the flux decreases by approximately 50%, while the maximum moves deeper into the SOL, further from the separatrix. The decrease of flux at the ISP is the consequence of the reduction of the parallel velocity, caused by the decrease of the electron and ion temperatures. This was also previously observed in single ion GBS simulations with increasing fuelling [68]. In contrast, the flux increases with density at the OSP, both in SOL and in the private flux regions, with a single peak centered inside the separatrix. This is due to a lower reduction of the parallel velocity at the OSP rather than the ISP, proportional to the ion temperature (see Fig. 4.8), combined with increased density due to the ionization reactions in the LFS, shown in Fig. 4.3.

The position of the flux peak can be explained by the increase in the $E \times B$ drift, resulting from the strong potential gradient close to both targets, shown in Fig. 4.9. In Fig. 4.12 we present the vector plot of the flux components on the poloidal plane, in the two simulations, where the colormap represents the vector module, while in Fig. 4.13 we present the sum of the three components.

In the low density simulation, the flux is dominated by the parallel component in the SOL and the $E \times B$ drift is only important inside the private flux region. While the parallel flux peaks close to the strike point, the $E \times B$ drift transports plasma from the OSP to the ISP. In the high density simulation, the contribution of the $E \times B$ drift increases, while the diamagnetic components in the poloidal plane are negligible. The drift creates a convective cell of circulating plasma, moving ions from above the X-point to the far SOL and from the OSP to the X-point, that modifies the transport balance between $\Gamma_{E \times B D^+}$ and $\Gamma_{\parallel D^+}$ differently at the two targets. In fact, with higher density the ion flux at the OSP peaks

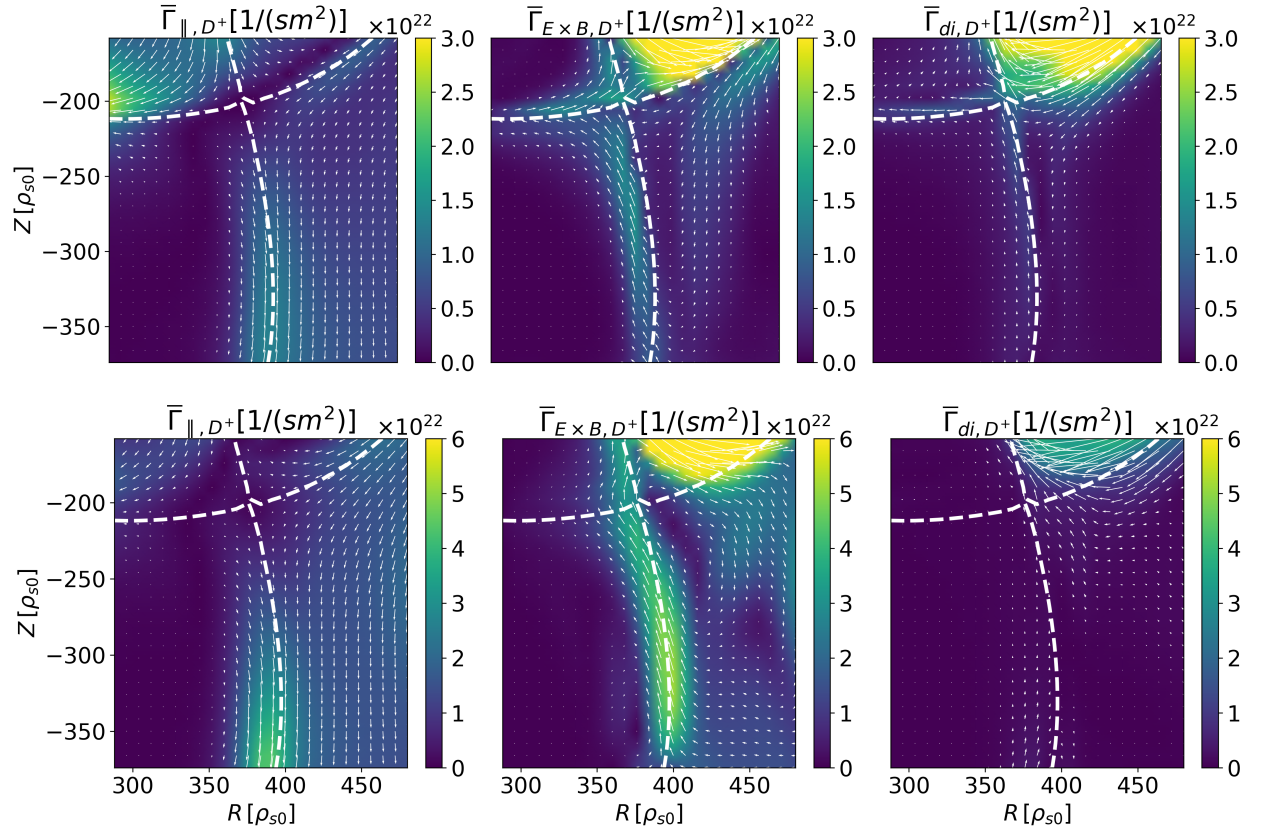


Figure 4.12: Vector plot of the average components of the ion flux projected on the poloidal plane, in the divertor volume, for the low density simulation (top row) and high density simulation (bottom row). The colormap represents the module of the vector.

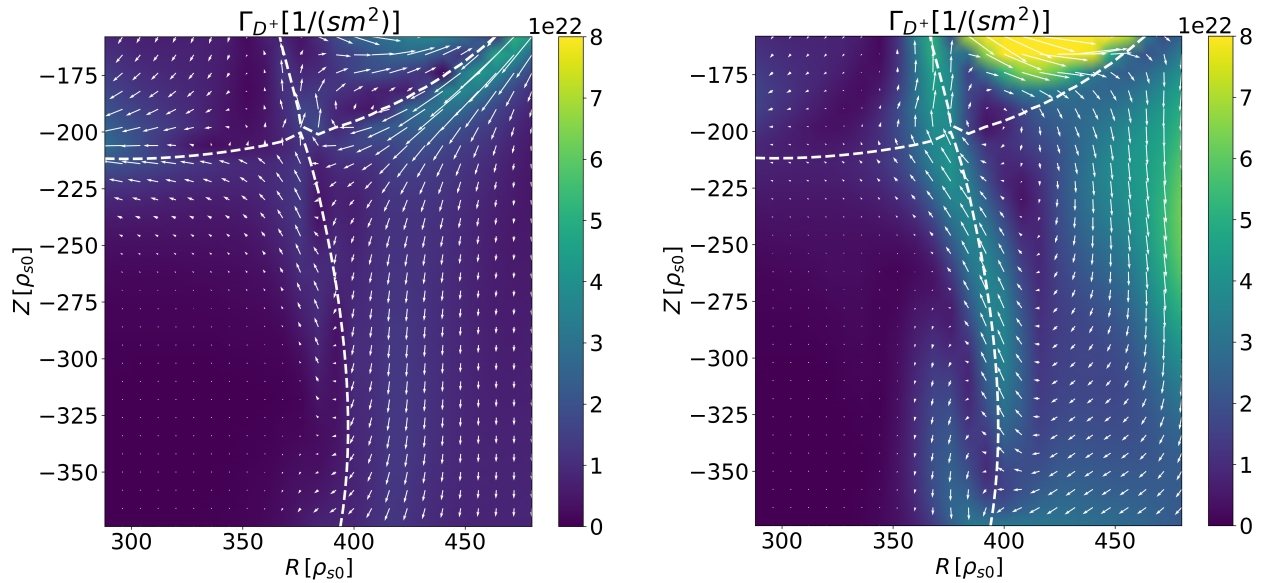


Figure 4.13: Vector plot of the total ion flux projected on the poloidal plane, in the divertor volume, for the low density simulation (left) and high density simulation (right). The colormap represents the module of the vector.

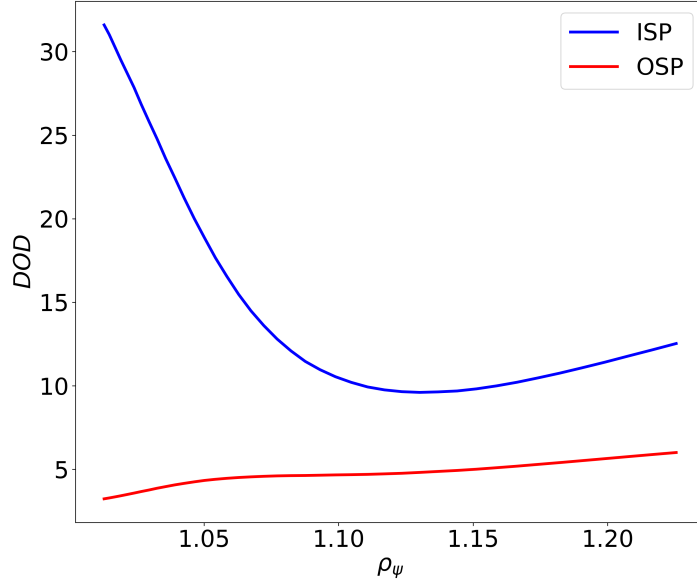


Figure 4.14: Degree of Detachment evaluated as $DOD = C n_{D+,up}^2 / \Gamma_{D+}$, for different flux tube positions, in the high density simulation.

inside the separatrix, at $\rho_\psi = 0.98$ in Fig. 4.11, while at the ISP the $E \times B$ drift moves the peak to $\rho_\psi = 1.12$.

In the high density simulation the decrease of the ISP particle flux is mainly caused by the decrease of ionization local sources with the reduction of parallel flux [68], while the contribute of the $E \times B$ drift to particle balance is small. Ultimately, the asymmetries between the target ion fluxes are generated by the asymmetries in the plasma-neutral interactions, see Fig. 4.6, and enlarged by the effect of the $E \times B$ drift [118, 111, 110], that is a consequence of the specific temperature profile set by molecular reactions.

4.3.2 Degree of Detachment

The two point model, derived to relate the evolution of the upstream profiles to the target density and temperature [12], establish quadratic dependence of the ion flux at the target from plasma density upstream, $\Gamma_{D+} \propto C n_{upD+}^2$. This model, validated in several devices, e.g. JET [106] or ASDEX [111], is valid for density below the detachment onset. Exploiting the two-point model results, the divertor recycling state is often characterized by the Degree Of Detachment (DOD), $DOD = C \frac{n_{upD+}^2}{\Gamma_{D+}}$. If $DOD > 1$ the measured flux at the target is lower than expected from the two-point model and the plasma is said to be detached. We note that the calibration constant C depends on the power crossing the separatrix and the connection length for the specific flux tube. In Fig. 4.14 we show the DOD profile of the high density simulation, for both targets, considering flux tubes positioned at different ρ_ψ . The two simulations we consider have the same input power in the SOL and the same magnetic geometry, therefore, we evaluate C from the low density simulation and use this value to establish if the high density simulation is in a detached state. This methodology is equivalent to consider the low density simulation as not detached, an hypothesis that gives us a lower limit on the DOD

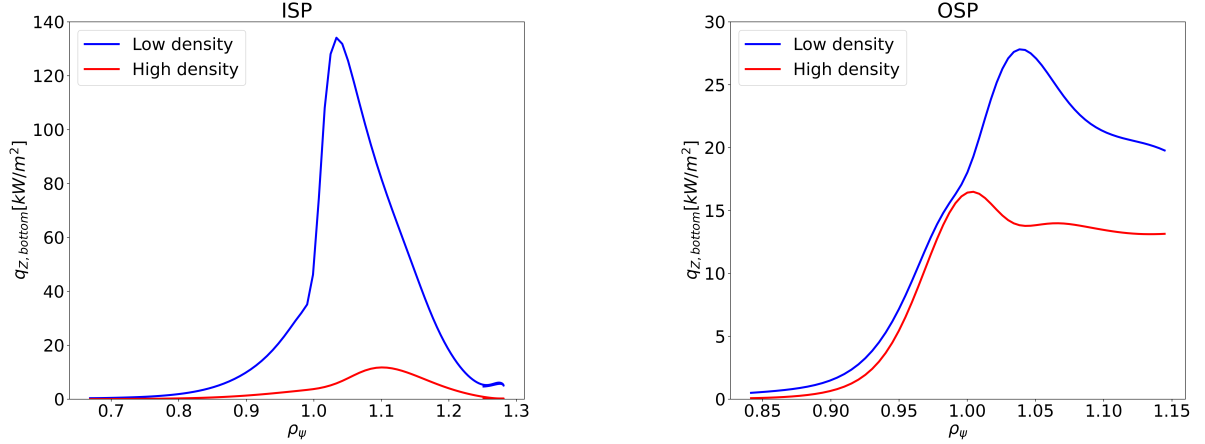


Figure 4.15: Average of the heat flux on the target, for both strike points, as a function of the normalized poloidal flux function.

value. The density upstream is evaluated as the average density at the separatrix at $Z = 0$. At the ISP we observe $\text{DOD} > 1$, across all the SOL region, as expected from the observed decrease of the ion flux. At the OSP we also observe $\text{DOD} > 1$, in particular at increasing distance from the separatrix, even if the ion flux is larger than the low density simulation. We can conclude that the high density simulation presents a detached ISP, comparable to the experimental conditions observed at density values larger than the ones necessary for the detachment onset, while the OSP is in a partially detached state, where the particle flux reduction is not observed [113].

4.3.3 Heat target flux

The time-averaged profiles of the heat flux for the two targets are shown in Fig. 4.15.

The pressure drop between OMP and divertor targets, together with the decrease of the target particle flux, yield a decrease of the heat flux at the targets. In GBS, we evaluate the sum of the D^+ ion and electron heat flux considering the contribution from conduction and convection due the parallel and drift fluxes

$$q_{\text{tot},j} = \frac{3}{2} T_{\text{D}^+} \Gamma_{\text{D}^+,j} - (\chi_{\perp,\text{D}^+} \nabla_{\perp,j} T_{\text{D}^+} + b_j \chi_{\parallel,\text{D}^+} \nabla_{\parallel} T_{\text{D}^+}) + \frac{3}{2} T_{\text{e}} \Gamma_{\text{e},j} - (\chi_{\perp,\text{e}} \nabla_{\perp,j} T_{\text{e}} + b_j \chi_{\parallel,\text{e}} \nabla_{\parallel} T_{\text{e}}), \quad (4.4)$$

where $\Gamma_{\text{D}^+,j}$ is defined in Eq. (4.3) and an analogous definition is used for Γ_{e} , the diffusion coefficients $\chi_{\perp}$ and $\chi_{\parallel}$ are those appearing in Eqs. (2.45 - 2.46) and b_j is the component of the magnetic field unit vector, with $j = R$ or Z . The D_2^+ contribution to the flux is neglected since $n_{\text{D}_2^+} \ll n_{\text{D}^+}$.

In the low density cases, heat flux is mainly determined by conduction and parallel electron convection, equally contributing with their sum accounting for 80% of the total heat flux. This leads to a heat flux peak located at the same position of the parallel ion flux both in the ISP and in the OSP. At high plasma density, the heat flux is lower at both targets, and it is flat at the ISP, in agreement with the pressure drop observed in Fig. 4.7. The contribution of D^+ ions,

largely dominated by convection, increases up to 40% of the total heat flux. As observed for the particle flux, the heat flux decrease is stronger for the ISP, due to the stronger reduction of parallel convection toward the target.

We point out that in our simulations we retrieve the experimental observations of heat flux decrease with the simultaneous increase of radiative and momentum losses upstream (see Fig. 4.6) at the onset of detachment [12, 15].

4.3.4 Mid-plane: density shoulder and turbulent transport

Experimental operation at high density achieved through the increase of gas throughput reveal the tendency to develop flatter density profiles generally associated with an increased level of turbulence, a phenomenon known as *density shoulder* [78, 102]. The simulations presented in Ch. 3, which do not include molecular interactions terms, show an increase of turbulence level and the flattening of the pressure profile with the increase of fuelling, modelled in past GBS simulations as the increase of atomic neutrals interactions [68] or with higher resistivity [95, 66].

We investigate the density shoulder formation also in the present sets of simulations. Density and pressure profiles for the two simulations considered in this work are shown in Fig. 4.16, normalized to their value at the separatrix. We identify two decay lengths, one in the near SOL, $1 \leq \rho_\psi \leq 1.1$, and one in the far SOL, in agreement with several experiments [122, 78] and simulations [66]. The increase of density yield an increase of the near SOL decay length, both for density and pressure. Similarly to the observation based on simulations including only atomic contribution [68], also in the present simulations the density shoulder appears in correspondence of a strong reduction of temperature and parallel flux at the target.

In order to estimate of the perpendicular transport we consider in Fig.4.17 the radial profiles at the OMP of the averaged $E \times B$ flux, $\bar{\Gamma}_{E \times B}$, of the effective transport coefficient, $D_{E \times B, \text{eff}} = \bar{\Gamma}_{E \times B} / |\nabla n_e|$, and of the effective velocity, $v_{E \times B, \text{eff}} = \bar{\Gamma}_{E \times B} / \bar{n}_e$. This includes both the time and toroidal averaged steady state and the fluctuating flux components of the $E \times B$ flux, $\bar{\Gamma}_{E \times B} = \Gamma_{\bar{E} \times \bar{B}} + \tilde{\Gamma}_{E \times B}$. In the SOL the fluctuating component accounts for half of the total flux in the low density simulation, while its relative importance increases in high density, up to 70% of the total flux. Both components are significantly larger than the diamagnetic flux, that will be neglected in this analysis. In the high density simulation $\Gamma_{E \times B}$ is larger compared to the low density case throughout the SOL, as expected from the higher density. The effective diffusion coefficient $D_{E \times B, \text{eff}}$ is also larger, pointing out that the actual transport associated with this flux is larger. The effective velocity, $v_{E \times B, \text{eff}}$, is larger in the high density simulation deep in the SOL, for $\rho_\psi > 1.15$. These results imply that the higher flux in the far SOL is not only an effect of the increased density, in contrast to the results of simulations that include only atomic deuterium in a simplified magnetic configuration [68].

Both experimental results and simulations show that the turbulent flux in a L-mode tokamak discharge in the far SOL is mostly the result of the movement of coherent filamentary structures, denoted as blobs. In GBS simulations, blobs are identified with an algorithm developed and used for the analysis of previous GBS results [96, 95], that was recently extended to detect their three-dimensional structure. The algorithm finds the regions where the density fluctuations are 2.5 times above the local standard deviation and tracks them in time. A fluctuation is identified as a blob if it is detected an area of at least $20\rho_{s0}^2$ on each plane and a toroidal extension above $\pi/5R_0$. The blob detection algorithm fits the density perturbation associated with a blob in the poloidal plane with a gaussian function. The full widths at half maximum in the radial and vertical direction are denoted as a_R and a_Z , respectively. From the blob center of mass motion, identified as the center of the fitting gaussian functions we retrieve the average blob velocities in the

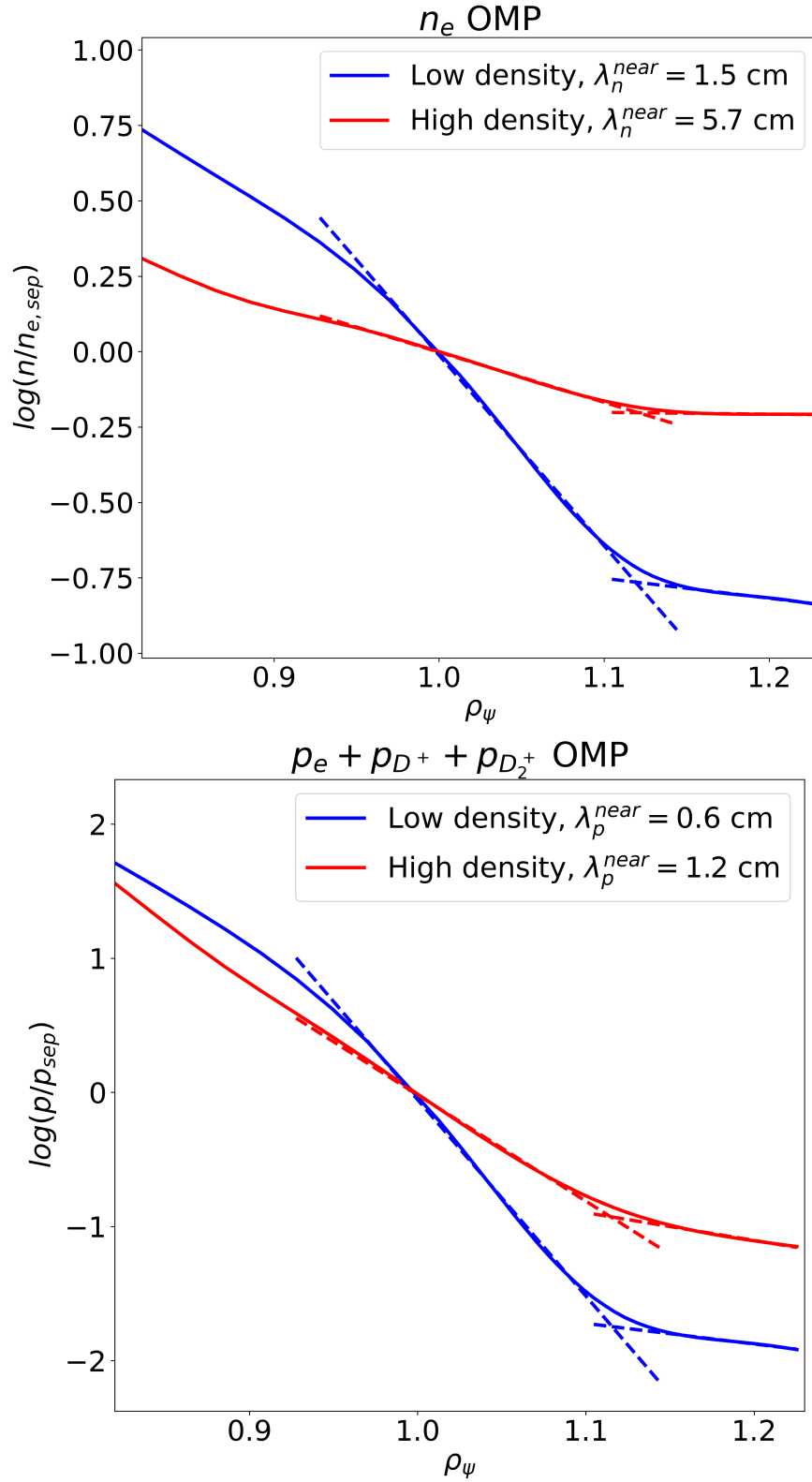


Figure 4.16: Average of the electron density and total plasma pressure at the OMP. In dashes the two linear fits that identify one decay length in the near SOL and another decay length in the far SOL.

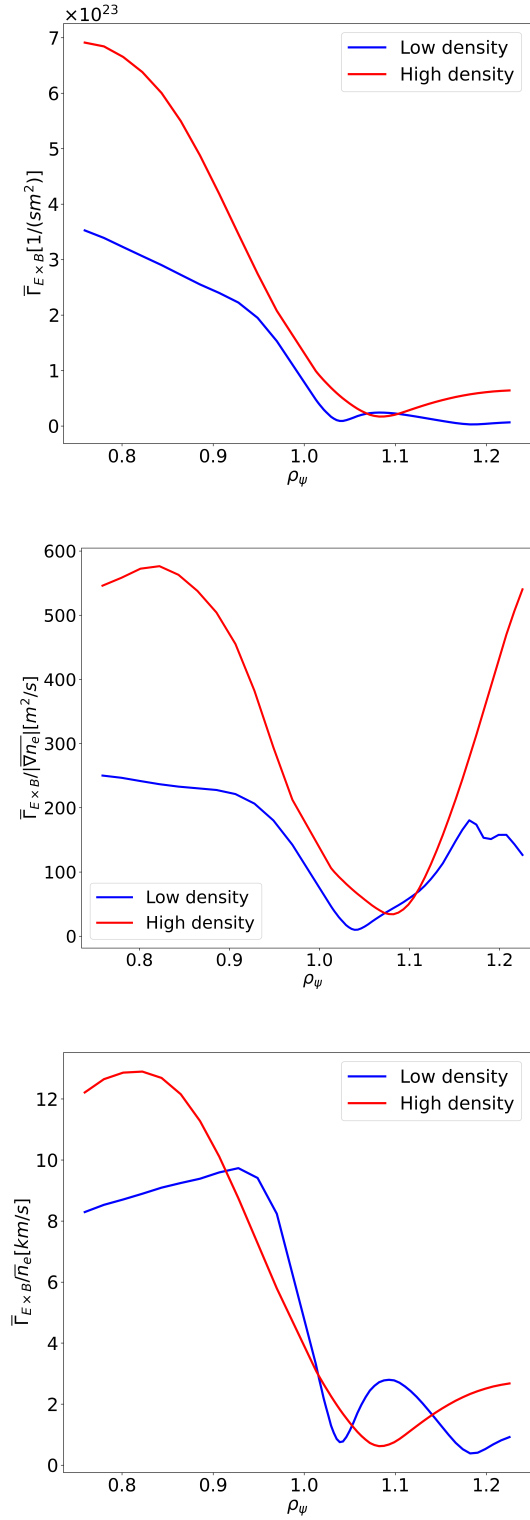


Figure 4.17: OMP profiles for the $\bar{\Gamma}_{E \times B}$ flux, the effective coefficient due to the $\Gamma_{E \times B}$ flux, $D_{E \times B, \text{eff}} = \bar{\Gamma}_{E \times B} / |\nabla n_e|$ and effective velocity $v_{E \times B, \text{eff}} = \bar{\Gamma}_{E \times B} / \bar{n}_e$.

poloidal plane, $v_{b,\psi}(R, Z)$ and $v_{b,\chi}(R, Z)$. Our analysis covers a time interval sufficiently large to ensure the statistical convergence of the blob properties.

In agreement with Ref. [66], blobs are typically in the RB conditions in our simulation, with bigger size for higher resistivity in the SOL [68], in agreement with experimental results [112]. In Fig. 4.18 we show the histograms of the blob radial velocity $v_{b,\psi}$ and size evaluated as $a_b = \sqrt{a_R a_Z}$. Our results reproduce the increase in average size and average radial blob velocity with increasing density and lowering resistivity, shown in dashes in figure 4.18.

In Fig. 4.19 the radial and poloidal components of the blob velocity, v_ψ and v_χ , are plotted at the OMP, as a function of the distance from the separatrix. The velocity v_ψ is normalised to the flux expansion f_x , since the radial velocity of a field-aligned structure is expected to be proportional to it, in agreement with experimental results [43]. At low density both the ratio v_ρ/f_x and v_χ increase with ρ_ψ in the near SOL and flatten in the far SOL, while in the high density simulation the blob velocity increases through the SOL. These trends are in qualitative agreement with experimental results, showing also the same order of magnitude for the average values [78, 112, 43]. The magnitude of blob's radial velocity is the same as the effective $v_{E \times B, \text{eff}}$ shown in Fig. 4.17, as expected [123, 43].

To compare the blob velocity distribution dependence on χ , we present the poloidal profile of the blob velocity components in Fig. 4.20, averaged over $\rho_\psi \geq 1.1$. We find higher radial velocity along all the SOL for higher density, while poloidal velocities are the same in the two simulations up to the X-point. Both in low and high density v_ψ and v_χ decrease for increasing χ , from the OMP to the X-point. Experimental measurements of the blobs velocities in TCV discharges, made at different distance from the X-point, show again the same trends as our simulation [124, 43].

To conclude, our blob tracking analysis results shows an increase in radial velocity with increasing fuelling, which leads to the larger turbulent $\Gamma_{E \times B}$ and to the larger effective perpendicular transport shown in Fig. 4.17. The increased perpendicular transport, together with the decreased parallel flux, yields a larger $\Gamma_\perp/\Gamma_\parallel$ ratio, going from $\Gamma_\perp/\Gamma_\parallel \simeq 0.05$ in the low density simulation to $\Gamma_\perp/\Gamma_\parallel \simeq 0.1$ with higher density. The increase of this ratio is ultimately responsible for the density shoulder formation [68, 89]. Compared to the single-ion simulations in Ch. 3, in these results we observe that the introduction of molecular interactions lowers the SOL plasma temperature, leading to higher resistivity and faster blobs [95], ultimately increasing the perpendicular transport and the ratio $\Gamma_\perp/\Gamma_\parallel$.

4.4 Conclusions

In this work we present the first multi-species simulations of plasma turbulence coupled to kinetic neutral dynamics, in a diverted configuration. The simulations are performed by exploiting the new version of the GBS code [37] and consider the magnetic equilibrium of a realistic TCV discharge, using the TCV-X21 equilibrium configuration [67]. The self-consistent treatment of the interactions between 5 species (electrons, D^+ and D_2^+ ions, D atoms and D_2 molecules) is simulated. The model takes into account the main collisional processes between plasma and neutrals, including ionization, recombination, elastic collisions, charge-exchange and molecular dissociation.

We present the results from two simulations performed at different fuelling rates, changing the amplitude of the gas puff of neutral D_2 . While GBS simulations that do not include the molecular dynamics retrieve important features associated with increased fuelling [68], the introduction of molecular dynamics improves the agreement with experimental results and the understanding of the processes at play in high-density L-mode tokamak discharges. For instance, the presence

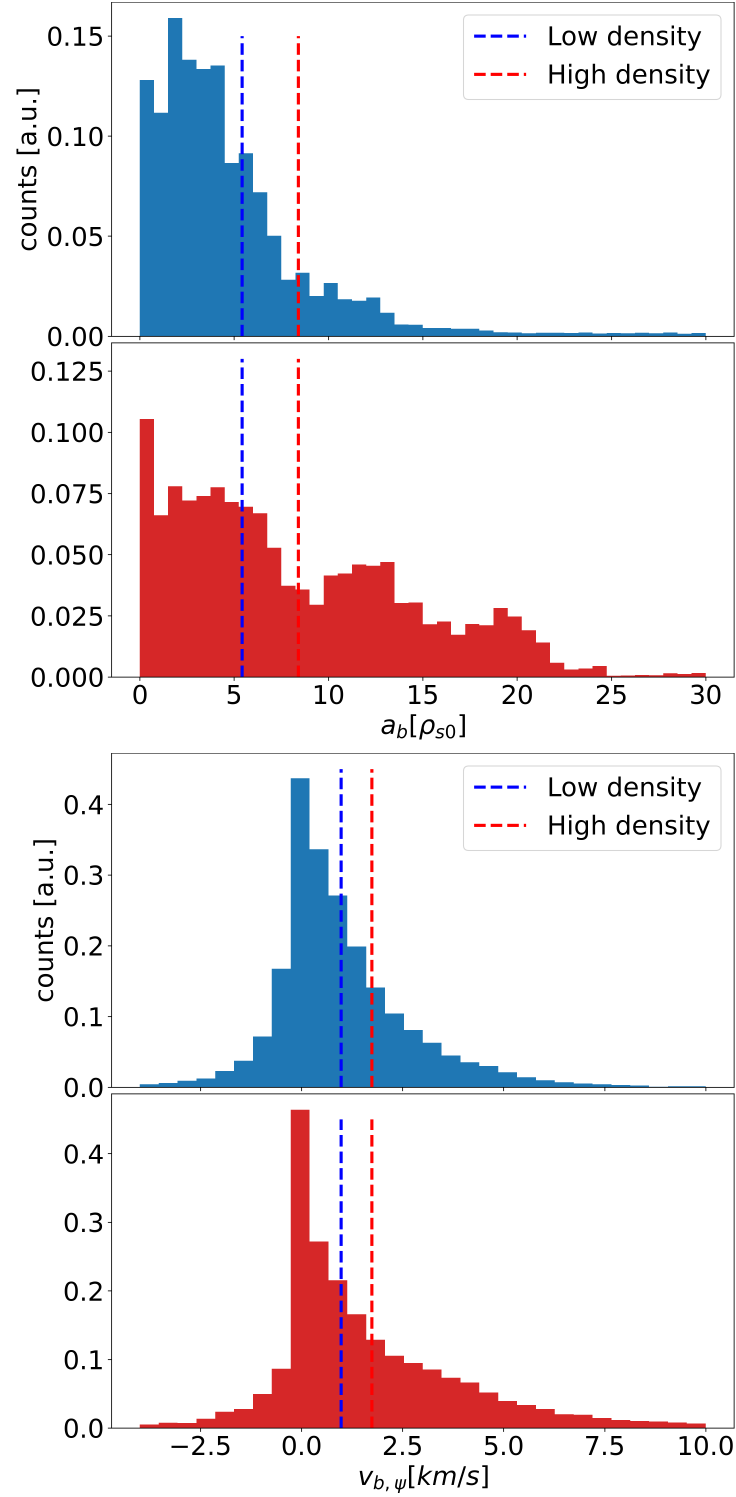


Figure 4.18: Histograms for blob's size $a_b = \sqrt{a_R a_Z}$ and radial velocity $v_{b,\psi}$ for all blobs. In dashes the average values, the counts are normalized to sum to 1.

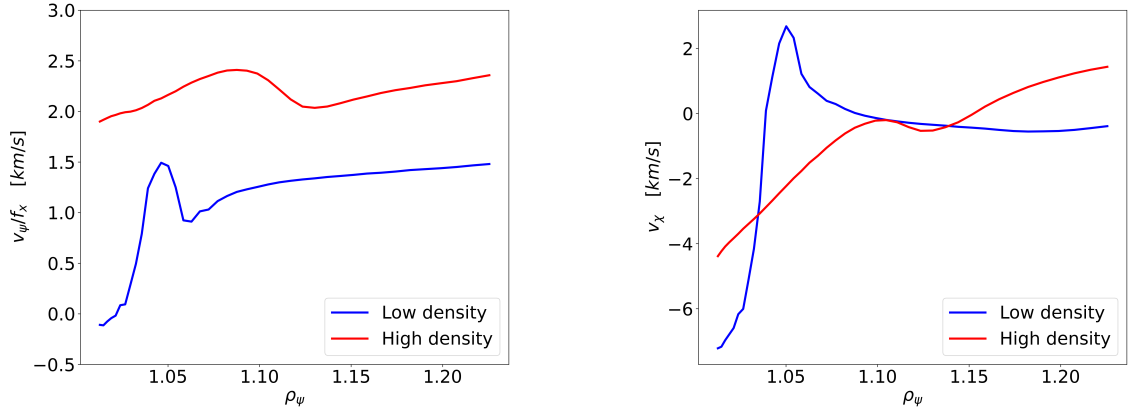


Figure 4.19: Blob's center of mass velocity components, radial ψ divided by the flux-expansion f_x and poloidal χ , averaged over all the blobs, for the OMP. The values are averaged over the OMP region.

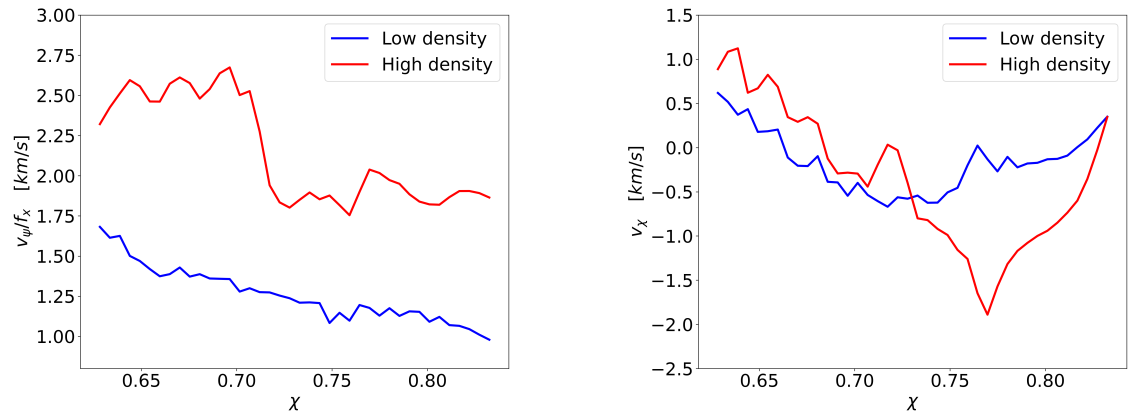


Figure 4.20: Blob's center of mass velocity components, averaged over all the blobs, in a flux tube in the far SOL $\rho_{\psi} \geq 1.1$. The values are expressed as a function of the poloidal coordinate χ , from the OMP, $\chi_{\text{OMP}} = 0.64$ to above the X-point $\chi_{\text{Xpt}} = 0.87$.

of a relevant density of D_2 activates new channels of D production, mainly MAR, producing atomic deuterium at a relatively high temperature, $T_{D,diss} \geq 3$ eV. The increase of the neutral density yield a large radiated power through ionization reactions, leading to power starvation in the divertor region and moving ionization from the targets to above the X-point. The high neutral density is also responsible for the increase of momentum losses, identified by the increase of charge-exchange reactions and the decrease of ion parallel velocity. For sufficiently low plasma temperature, $T_e < 3$ eV, molecular dissociation and charge-exchange between D^+ and D become the main plasma energy sink, leading the ion and electron temperatures to values close to the neutral temperature $0.03 \text{ eV} < T_D < 3 \text{ eV}$.

Because of the low temperature values and associated momentum losses, the parallel ion velocity is reduced in high density with respect to low density simulations as observed in previous GBS simulations [68]. This yield a reduction of total heat flux at the targets, lowering both heat convection and heat conduction. In particular, the increase in fuelling causes a strong reduction of particle flux at the ISP, compatible to typical experimental observations in the detachment regime. Indeed, to our knowledge, the simulations presented in this work are the first simulations of plasma detachment that include a self-consistent treatment of plasma turbulence and neutral interactions. The particle balance analysis conducted in this work shows that the decrease of the flux to the wall in the high density simulation, associated with a decreased ionization source, is due to a reduced plasma temperature in the SOL. The asymmetries between the ISP and OSP are explained by the different local plasma temperature and molecular neutral density, in turn determined by the magnetic configuration and by the position of the gas puff, combined with the effect of a strong $E \times B$ flux.

In addition, the reduced plasma temperature leads to an increase of the plasma resistivity. This generates strong electric field in the SOL. In fact, the equilibrium profile of the parallel electric field $E_{||}$ follows the generalized Ohm's law, in Eq. (4.2), where the contributions of the electron temperature and pressure gradients are negligible compared to the resistive term, $\nu j_{||}$. This results in higher $\Gamma_{E \times B}$ with higher fuelling, increasing plasma density in the private flux region at the bottom target, and increasing radial transport from the core to the wall at the mid-plane.

The profiles of both density and pressure at the OMP show that the increase in fuelling leads to the formation of a density shoulder and an increase of the near SOL decay length for both quantities. We confirm that the density shoulder is the result of an increase of the perpendicular transport together with the decrease of parallel transport. Leveraging blob tracking routines developed in past studies and recently improved, we perform a detailed investigation of filamentary transport in the SOL, comparing blob velocities with the $\bar{v}_{E \times B}$. We observe an increase of blob radial velocity with increased fuelling, well reproduced by the increase in the $v_{E \times B}$ due to stronger electric field in the far SOL. It is interesting to notice that the increase in radial velocity was not observed in simulations where fuelling was increased without molecules and the plasma temperature in the far SOL was higher [68].

From the analysis of our simulation we retrieve several qualitative similarities with experimental results. For instance, the increase of deuterium puffing leads to a decrease in the particle and heat flux at the targets, detachment conditions at one of the targets [12, 106]. The asymmetry between the two targets results from the combination of local D_2 and D_2^+ density [110] and stronger $E \times B$ drift [111]. Our results of filamentary transport reproduce the increase of radial velocity at higher density [112, 43], where faster blobs appears in correspondence of a strong electric field in the SOL, determined by plasma resistivity at low temperature. This result shows the necessity of a specific experimental analysis of the SOL electric field in high density simulations, extending the first results recently obtained in L-mode discharges [119].

5 Conclusions

The implementation of a new multi-component, self-consistent plasma and neutral model has been carried out during this PhD project, together with its application to simulate L-Mode Single Null Divertor (LSN) configurations. Leveraging on the new capabilities of the GBS code, able to approach different turbulent regimes with different filamentary transport dynamics [66, 97], the present thesis focused on the study of plasma-neutral interaction exploring the modification of SOL profiles and fluctuations at increased plasma fuelling. Accurate understanding of high-density operational regimes, while keeping acceptable heat and particle flux toward the Plasma Facing Components, are indeed of fundamental interest for the development of efficient fusion reactors. The novel model, implemented in the present thesis, allowed to explore precedently uncovered high density scenarios, reaching condition of divertor detachment, an operational scenarios foreseen for future devices.

Ch.2 describes the latest version of the GBS model, including the derivation of the multi-species plasma fluid equations and the resolution of the neutral's kinetic equations. The plasma equations are based on a set of drift-reduced Braginskii equations for electrons and ions, that implements the Zhdanov closure. The neutral model solves two kinetic Boltzmann equations in order to find neutral's density, velocity components and temperature. In the model, plasma and neutrals can interact through several collisional processes, including ionization, recombination, charge-exchange and molecules dissociation. Each of these reactions introduces specific terms in the evolution of the plasma and neutral profiles. While the methodology can be applied to any kind of species, we applied it to a deuterium plasma composed by atoms and molecules, in order to address physical scenarios which are relevant in high density detached plasma [125, 126, 40] or can be as well useful for diagnostic purpose [46]. The model is implemented in the version of the code that encompasses the full tokamak volume, retaining the core-edge-SOL interplay and using non-field aligned coordinates to handle divertor geometries.

In ch.3 we present the first study carried out with GBS simulations in diverted configuration with self-consistent kinetic neutrals, aimed to understand the mechanisms behind the flattening of the density mid-plane profile when core fuelling is increased, i.e. the process known as *density shoulder* formation [41]. We reconstruct a turbulent quasi-steady state for a plasma composed by one ion species interacting with one neutral species, namely deuterium, in a TCV-like LSN discharge. In particular we compare simulations with neutral interaction included and increasing core fuelling, with

others without neutrals, where the density source is artificially modified to match the same separatrix density. Before the introduction of self-consistent neutral interactions, it was already possible to reproduce the density shoulder through an increase in the plasma resistivity [81]: however, in our simulation, we reproduce this results by increasing neutral density and, consequently, core fuelling. In particular, we recover higher densities in the far SOL, together with reduced electron temperature and higher resistivity at the LCFS, due to the increase of ionization reactions above the X-point. The process of the shoulder formation is investigated by considering a global particle balance in the SOL, including parallel and perpendicular transport as well as local ionization. From the outcome of the simulations we conclude that the reduction of parallel flux, due to lower target temperature, is leading to higher densities in our simulations, with a minor contribution from the increase of local density sources in the SOL and the changes in the perpendicular flux. The perpendicular flux is analyzed in details, characterizing the blobs of our simulation and measuring their velocity and size. With increasing fuelling, we observe an increase in the blob size, in agreement with previous numerical studies [127] and experimental results [78]. Nevertheless, we observe a reduction of the perpendicular flux caused by a reduction of blob's radial velocity. Consequently, as detailed in [68], these set of simulations suggested the process of density shoulder primarily due to a reduction of the parallel transport with consequent increase of the ration $\Gamma_{\perp}/\Gamma_{\parallel}$.

The full model, describing a deuterium plasma composed by 5 different species (e^{-} , D^{+} , D_2^{+} , D and D_2), has been then exploited, with the aim to provide a self-consistent simulation of a detached plasma as described in Ch. 4. In particular, with the complete model we have been able to analyze the influence of molecular interactions in the quasi-steady state plasma transport and turbulence, in a TCV-like tokamak discharge, in conditions compatible with plasma detachment. For this purpose we used the so-called TCV-X21 [67] scenarios, a LSN L-mode plasma at reduced toroidal field ($B_{\varphi} = 0.9T$), previously used as for a multi-code validation exercise at low density [67]. We performed a set of simulation with increasing fuelling, where now the magnetic configuration is retrieved from an experimental discharge and fuelling is modelled by D_2 puffing. The additional simulation of processes involving molecular dynamics, allowed to reconstruct with higher accuracy neutral emission by Franck-Condon dissociation and the plasma dynamic at low temperatures $T_e \leq 3eV$. We find that molecular activated recombination is the main mechanism of D neutral production, fundamental to determine n_D and T_D in the divertor volume, close to the inner and outer strike points. Collisions between plasma and neutrals act as energy sinks for the plasma, in a different way accordingly to the different plasma density and temperature explored. While with only D neutrals ionization losses dominates in the SOL, the introduction of molecules leads to a strong local increase in n_D , decreasing ionization in the divertor region and increasing the energy loss due to molecular dissociations and charge-exchange. The increase in charge-exchange reactions guarantees the presence of a momentum loss mechanism, that, together with the radiative energy losses, is fundamental to sustain low target fluxes and a strong pressure drop between mid-plane and targets [12]. Simulations results show that the increase of molecular reactions leads indeed to higher pressure drops, together with decreased inner target particle flux and heat flux. The decrease of particle flux with increased upstream plasma density results in a stronger detachmend as measured by the so-called Degree Of Detachment. An analysis of the particle balance shows that the main reason for the flux decrease is lower parallel transport, together with a minor contribution from the lower local ionization. The perpendicular flux in the divertor region is dominated by the $E \times B$ flux, higher for higher n_{D_2} . Low temperature value in the SOL leads to higher resistivity and to strong electric fields in the far SOL, where the main contribution to the generalized Ohm's law is due to the resistive term $\nu j_{\parallel}$. This is a clear difference from other modelling results, where in higher plasma temperatures the contribute by plasma resistivity can be neglected [119], showing that the role of neutrals in determining the local plasma temperature can be fundamental to understand plasma transport. As a consequence of the different electric field at the OMP we observe an increase of turbulent flux, primarily due to an increase of the

blob size and radial velocity. While bigger blobs were observed also in simulations without molecules, the increase of radial velocity is a novelty introduced by the peculiar profile of the plasma temperature and the electric field at the OMP, responsible for higher $E \times B$ local velocities. The effect of higher $E \times B$ flux in the outer divertor volume is the increase of plasma density inside the separatrix, close to the target, and toward the X-point. We remark that the $E \times B$ direction is determined by the direction of the toroidal magnetic field, ion- ∇B drift pointing from the core toward the X-point in our simulation. The effect of an opposite B_ϕ will be investigated in future works. Ultimately, we find that the introduction of proper molecular physics in our model leads to conditions close to the detachment observed in experiments, retrieving several qualitative similarities with experiments. The asymmetries between the two targets can be explained by asymmetries in n_{D_2} and $n_{D_2^+}$, that determines differences in the collisional processes and in plasma temperature, leading to decreasing parallel fluxes and increasing $E \times B$ drifts differently for the two targets.

The results of our simulations represents a step forward toward more accurate simulations of plasma turbulence in the boundary of tokamak devices. We would like to remark that the use of a kinetic model for the neutral dynamics, like implemented in GBS, introduces a promising way to simulate the interplay between plasma and neutrals also in complex configurations and with different species. In the near future the neutral model will be improved, e.g. relaxing the hypothesis of neutrals confined in single poloidal planes and improving the performance of the code, in order to allow simulations including more than two species. This effort will go in parallel with the improvement of the entire GBS code. In the near future GBS will soon be ported on GPU, strongly reducing the time necessary to run a simulation, together with an improved capabilities to handle flexible wall geometry. All those improvements are fundamental to run simulations of configurations relevant for ITER and DEMO, in order to understand the physics of plasma turbulence with realistic parameters.

A List of kernel functions

The kernels appearing in Eqs. (2.74-2.77), used to evaluate n_{D_2} , Γ_{out,D_2} , n_D and $\Gamma_{out,D}$, are defined as the sum of the contribute of all the possible paths that connects the point at coordinate $\mathbf{x}_\perp$ to $\mathbf{x}'_\perp$, like in Eq. (2.78). For the single path, each kernel function includes the integral of a different velocity distribution for the different neutral emission processes. The list of resulting kernels is

$$K_{p \rightarrow p, path}^{D_2, D_2^+}(\mathbf{x}_\perp, \mathbf{x}'_\perp) = \int_0^\infty \frac{1}{r'_\perp} \Phi_{\perp} \left[\mathbf{v}_{\perp, D_2^+}, T_{D_2^+} \right] (\mathbf{x}'_\perp, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} \nu_{eff, D_2}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp, \quad (A.1)$$

$$K_{b \rightarrow p, path}^{D_2, reem}(\mathbf{x}_\perp, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_\perp}{r'_\perp} \cos \theta' \chi_{\perp, in, D_2}(\mathbf{x}'_{\perp b}, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} \nu_{eff, D_2}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp, \quad (A.2)$$

$$K_{b \rightarrow p, path}^{D_2, refl}(\mathbf{x}_\perp, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{1}{r'_\perp} \Phi_{\perp} \left[\mathbf{v}_{refl(D_2^+)}, T_{D_2^+} \right] (\mathbf{x}', \mathbf{v}) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} \nu_{eff, D_2}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp, \quad (A.3)$$

$$K_{p \rightarrow b, path}^{D_2, D_2^+}(\mathbf{x}_{\perp b}, \mathbf{x}'_\perp) = \int_0^\infty \frac{v_\perp}{r'_\perp} \cos \theta \Phi_{\perp} \left[\mathbf{v}_{\perp, D_2^+}, T_{D_2^+} \right] (\mathbf{x}'_\perp, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} \nu_{eff, D_2}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp, \quad (A.4)$$

$$K_{b \rightarrow b, path}^{D_2, reem}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_\perp^2}{r'_\perp} \cos \theta \cos \theta' \chi_{\perp, in, D_2}(\mathbf{x}'_{\perp b}, \mathbf{v}_\perp) \exp \left[-\frac{1}{v_\perp} \int_0^{r'_\perp} \nu_{eff, D_2}(\mathbf{x}''_\perp) dr''_\perp \right] dv_\perp, \quad (A.5)$$

Appendix A. List of kernel functions

$$K_{b \rightarrow b, \text{path}}^{\text{D}_2, \text{refl}}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp} \left[\mathbf{v}_{\perp, \text{refl}(\text{D}_2^+), T_{\text{D}_2^+}} \right] (\mathbf{x}', \mathbf{v}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}_2}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.6})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{D}^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}^+, T_{\text{D}^+}}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.7})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{D}_2^+}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}_2^+}}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.8})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{diss}(\text{D}_2^+)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}, \text{diss}(\text{D}_2^+)}}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.9})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{diss-rec}(\text{D}_2^+)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}, \text{diss-rec}(\text{D}_2^+)}}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.10})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{diss}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}_2}, T_{\text{D}, \text{diss}(\text{D}_2)}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.11})$$

$$K_{p \rightarrow p, \text{path}}^{\text{D}, \text{diss-iz}(\text{D}_2)}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{D}_2}, T_{\text{D}, \text{diss-iz}(\text{D}_2)}] (\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.12})$$

$$K_{b \rightarrow p, \text{path}}^{\text{D}, \text{reem}}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta' \chi_{\perp, \text{in}, \text{D}}(\mathbf{x}'_{\perp b}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.13})$$

$$K_{b \rightarrow p, \text{path}}^{\text{D}, \text{refl}}(\mathbf{x}_{\perp}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{1}{r'_{\perp}} \Phi_{\perp} [\mathbf{v}_{\perp, \text{refl}(\text{D}^+), T_{\text{D}^+}}] (\mathbf{x}', \mathbf{v}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.14})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{D}^+}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}^+, T_{\text{D}^+}}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.15})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{D}_2^+}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}_2^+}}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.16})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{diss}(\text{D}_2^+)}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}, \text{diss}(\text{D}_2^+)}}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.17})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{diss-rec}(\text{D}_2^+)}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}_2^+, T_{\text{D}, \text{diss-rec}(\text{D}_2^+)}}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.18})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{diss}(\text{D}_2)}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}_2}, T_{\text{D}, \text{diss}(\text{D}_2)}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.19})$$

$$K_{p \rightarrow b, \text{path}}^{\text{D}, \text{diss-iz}(\text{D}_2)}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\perp, \text{D}_2}, T_{\text{D}, \text{diss-iz}(\text{D}_2)}](\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.20})$$

$$K_{b \rightarrow b, \text{path}}^{\text{D}, \text{reem}}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_{\perp}^2}{r'_{\perp}} \cos \theta \cos \theta' \chi_{\perp, \text{in}, \text{D}}(\mathbf{x}'_{\perp b}, \mathbf{v}_{\perp}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}, \quad (\text{A.21})$$

$$K_{b \rightarrow b, \text{path}}^{\text{D}, \text{refl}}(\mathbf{x}_{\perp b}, \mathbf{x}'_{\perp b}) = \int_0^\infty \frac{v_{\perp}}{r'_{\perp}} \cos \theta \Phi_{\perp}[\mathbf{v}_{\text{refl}(\text{D}^+)}, T_{\text{D}^+}](\mathbf{x}', \mathbf{v}) \exp \left[-\frac{1}{v_{\perp}} \int_0^{r'_{\perp}} \nu_{\text{eff}, \text{D}}(\mathbf{x}''_{\perp}) dr''_{\perp} \right] dv_{\perp}. \quad (\text{A.22})$$

We remark that all velocity distributions are a Maxwellian or a Knudsen cosine law, that is integrated along the parallel velocity:

Appendix A. List of kernel functions

$$\Phi_{\perp[\mathbf{v}^*, T^*]}(\mathbf{x}'_{\perp}, \mathbf{v}_{\perp}) = \int_0^{\infty} \Phi_{[\mathbf{v}^*, T^*]}(\mathbf{x}'_{\perp}, \mathbf{v}) dv_{\parallel} = \int_0^{\infty} \left(\frac{m_e}{2\pi T^*} \right)^{3/2} \exp \left(-m_e \frac{(\mathbf{v} - \mathbf{v}^*)^2}{2T^*} \right) dv_{\parallel}, \quad (\text{A.23})$$

$$\chi_{\perp, \text{in}}(\mathbf{x}'_{\perp, b}, \mathbf{v}_{\perp}) = \int_0^{\infty} \chi_{\text{in}}(\mathbf{x}'_{\perp, b}, \mathbf{v}_{\perp}) dv_{\parallel} = \int_0^{\infty} \frac{3}{4\pi} \frac{m_n^2}{T_b^2} \cos(\theta) \exp \left(-m_n \frac{|\mathbf{v}|^2}{2T_b} \right) dv_{\parallel}, \quad (\text{A.24})$$

where v^* and T^* are the velocity and temperature appearing in the previous equations, m_n is the mass of D or D₂, θ is the angle between $\mathbf{v}$ and the perpendicular to the wall and T_b is the wall temperature.

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