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Development of a Deuterium Plasma Global Model for Fusion- Relevant Applications

**TESI DI LAUREA MAGISTRALE IN
NUCLEAR ENGINEERING - INGEGNERIA NUCLEARE**

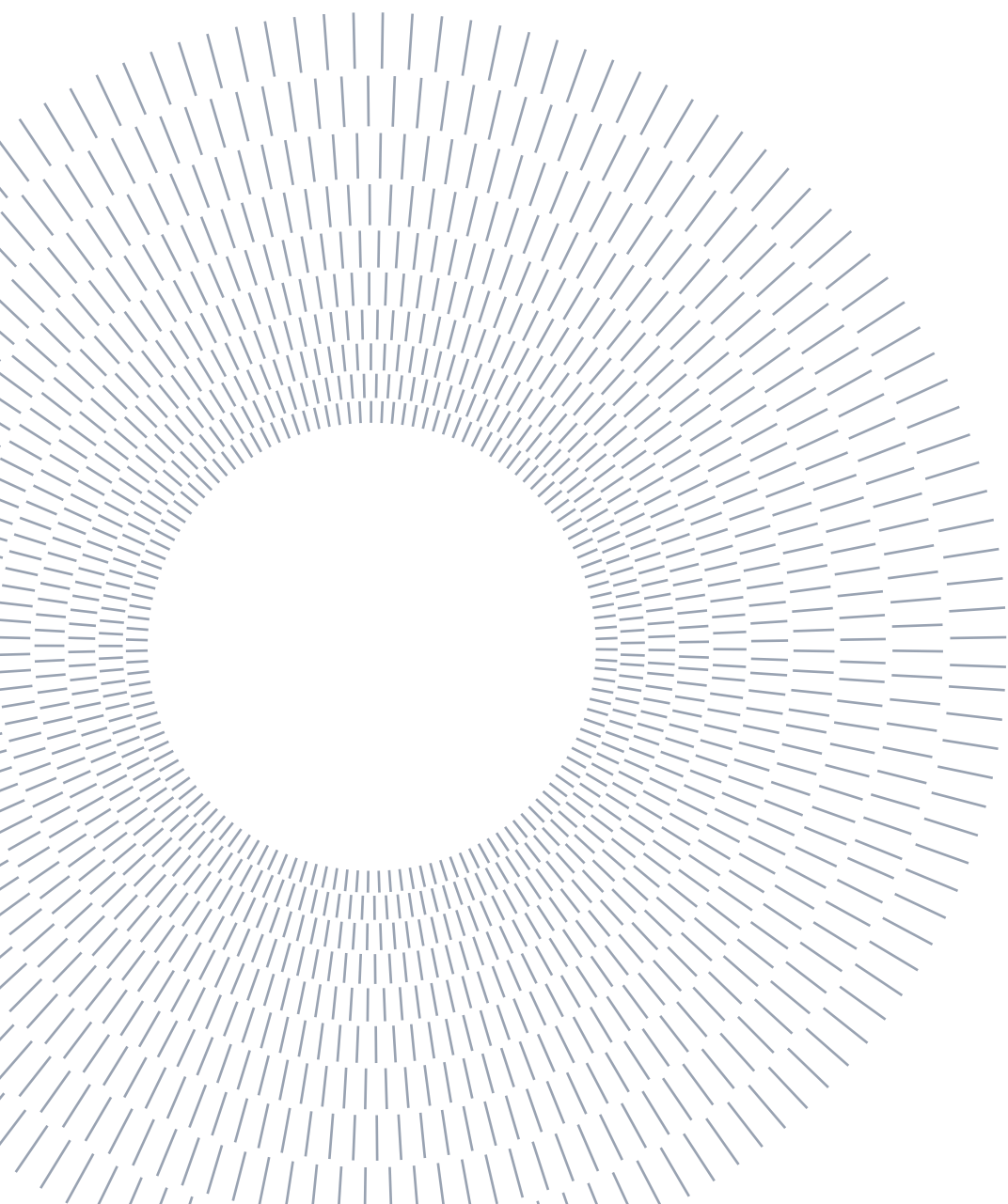
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Abstract

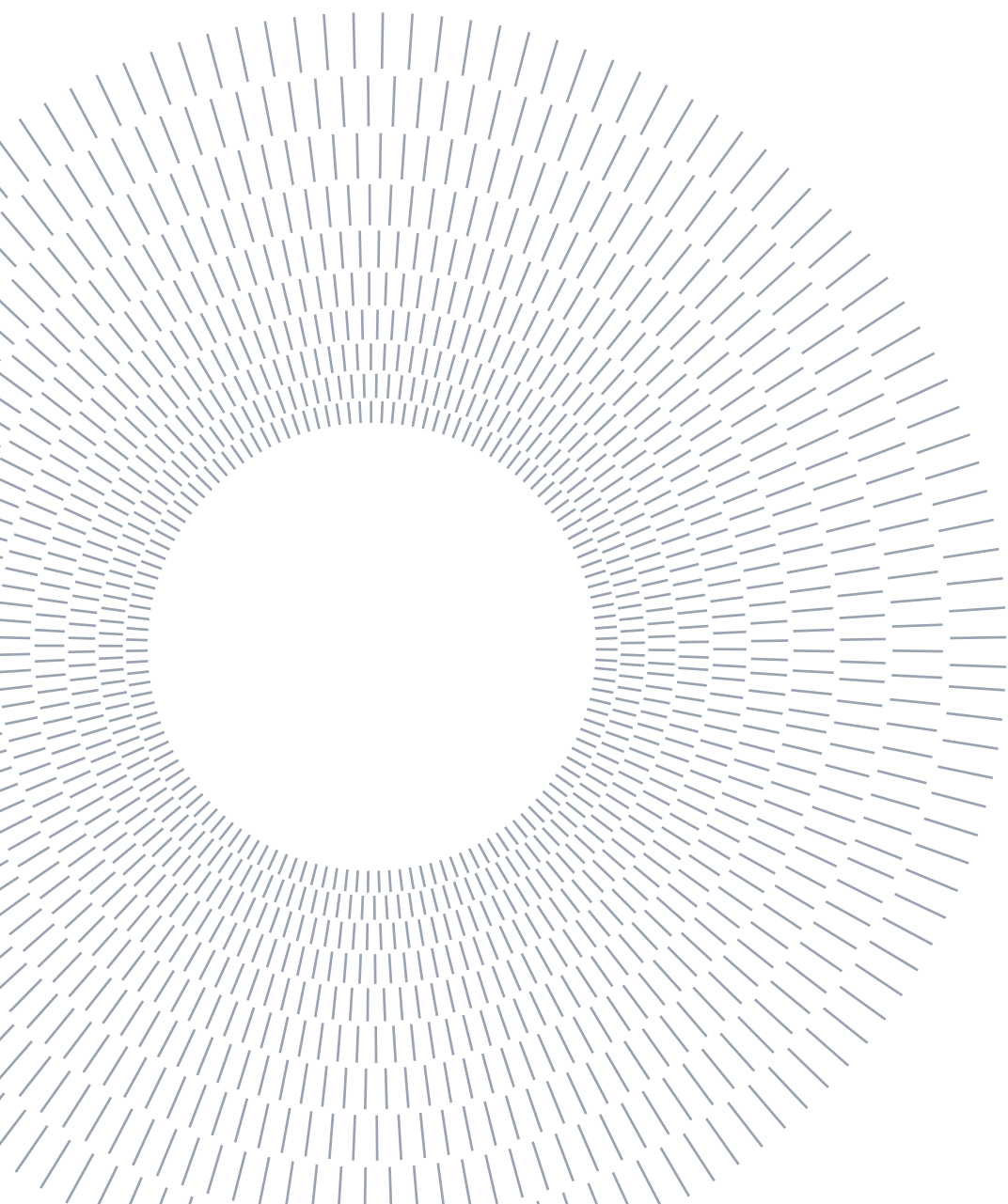
Hydrogen plasmas are central to fusion research, with the Deuterium-Tritium reaction as the most promising candidate for future fusion reactors. However, their molecular nature gives rise to considerable physical and chemical complexity. In this context global (0D) models provide an efficient framework to capture the interplay of numerous reactions at modest computational cost. They are particularly suitable for application to Linear Plasma Devices (LPDs), where an accurate prediction of plasma composition is essential for plasma-material interaction studies. Global models also help identify missing physics and inadequate assumptions in higher-fidelity models. However, dedicated isotopic adaptations of hydrogen 0D models are still lacking.

This thesis aims to develop a global model specifically for deuterium plasmas and to apply it to the investigation of deuterium plasmas in the GyM LPD, together with the validation of its predictions against experimental observations. In addition, it addresses open questions regarding the validity of the SOLPS-ITER modeling approach for molecular ions in LPDs through comparison with the developed 0D model.

The model is first developed for hydrogen to enable benchmarking against reference cases from the literature, showing good agreement and thereby demonstrating its predictive capability. Comparison with GyM experimental data confirms the reliability of its deuterium adaptation and its ability to provide valuable insight into the plasma composition, which is shown to be dominated by molecular ions. Finally, comparison between the 0D model and the SOLPS-ITER results indicates that the treatment of molecular ions in the latter should be revised under the considered operating conditions.

The developed model proved to be a reliable and effective tool for the investigation of low-temperature and low-to-intermediate pressure hydrogenic plasmas. Moreover, it demonstrated its value in complementing SOLPS-ITER and higher-fidelity models in general.

Keywords: nuclear fusion, deuterium plasmas, global models, SOLPS-ITER, linear plasma devices



Abstract in lingua italiana

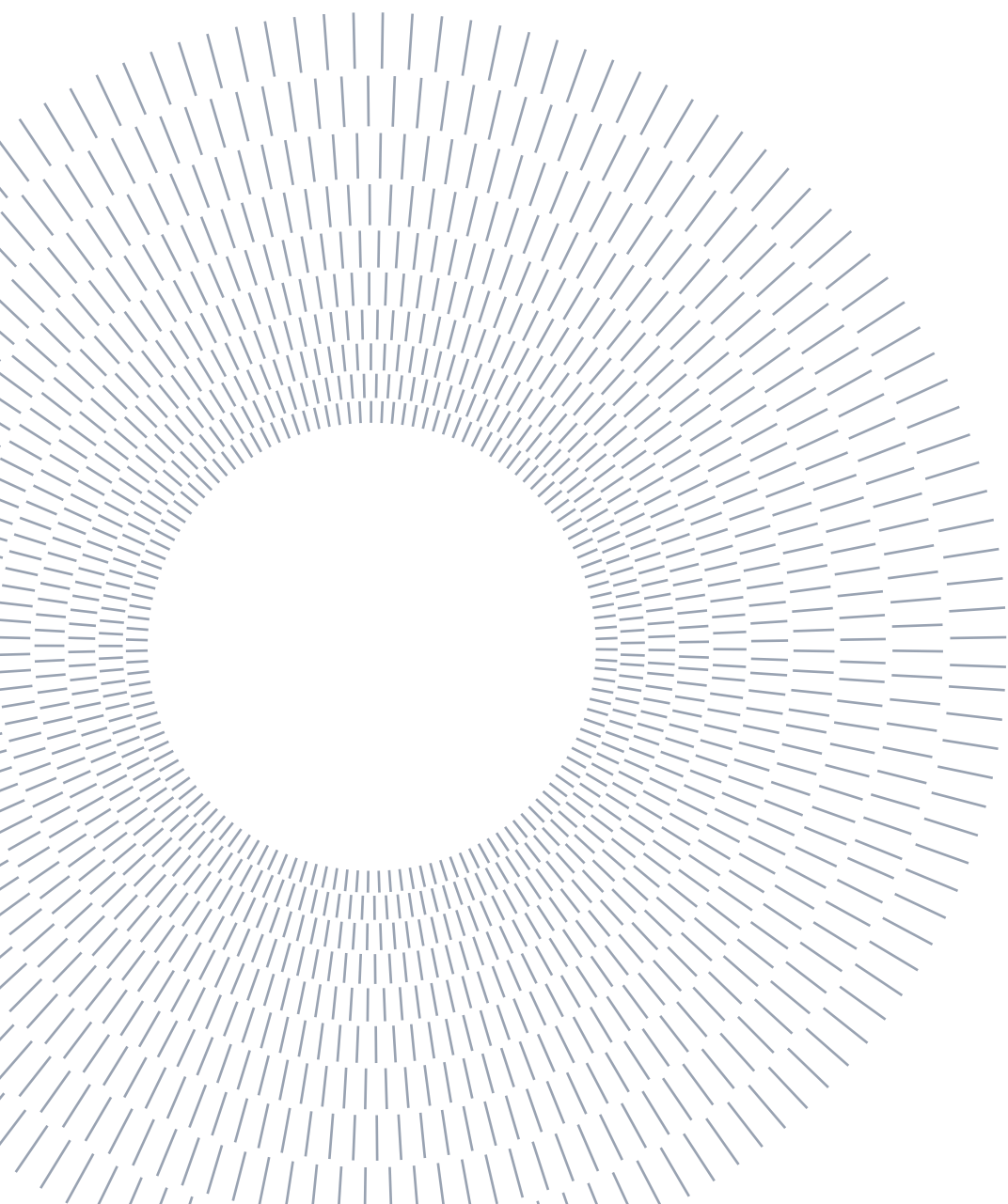
I plasmi di idrogeno sono centrali nell'ambito della ricerca sulla fusione, in cui la reazione tra Deuterio e Trizio è considerata la più promettente per lo sviluppo di un futuro reattore. Tuttavia, a causa della loro natura molecolare, sono caratterizzati da un'elevata complessità chimica e fisica. In questo contesto, i modelli globali (0D) si rivelano uno strumento efficace per riprodurre l'interazione tra numerose reazioni a fronte di un costo computazionale modesto. Sono particolarmente adatti ad essere applicati a dispositivi a plasma lineari, in cui accurate stime della composizione del plasma sono essenziali per studi di interazione plasma-materia. I modelli globali sono anche utili nell'individuare assunzioni inadeguate o mancanti in modelli più accurati. Tuttavia sono carenti in letteratura gli adattamenti di modelli 0D di plasmi di idrogeno ai suoi isotopi.

Questa tesi mira a sviluppare un modello globale specifico per plasmi di deuterio e ad applicarlo allo studio di plasmi di deuterio nella macchina lineare GyM, svolgendo al contempo un'attività di validazione del modello stesso. Inoltre, attraverso il confronto con il modello 0D, si vuole affrontare il tema della validità dell'approccio modellistico di SOLPS-ITER per ioni molecolari nei dispositivi lineari.

Il modello è stato inizialmente sviluppato per l'idrogeno, al fine di effettuare un confronto diretto con modelli di letteratura, il quale ha dimostrato ottimi risultati. Il confronto con i dati sperimentali di GyM ha confermato l'affidabilità del modello anche rispetto al suo adattamento al deuterio, fornendo in aggiunta importanti informazioni sulla composizione del plasma che è risultato essere dominato da ioni molecolari. In fine il confronto tra il modello 0D e SOLPS-ITER ha indicato che il trattamento degli ioni molecolari in quest'ultimo dovrebbe essere rivisto almeno per le condizioni operative indagate.

Il modello sviluppato ha dimostrato di essere affidabile ed efficace nello studio di plasmi idrogenoidi a bassa temperatura e pressione bassa-intermedia. Inoltre si è rivelato un valido strumento complementare rispetto a modelli più accurati come SOLPS-ITER.

Parole chiave: fusione nucleare, plasmi di deuterio, modelli globali, SOLPS-ITER, dispositivi a plasma lineari



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1 | Introduction

According to the International Energy Agency (IEA) [1], global energy demand has increased by nearly 60% since 2000, largely driven by emerging markets and developing economies, and it continues to grow steadily year by year. In response to the objectives of the 2015 Paris Agreement aimed at reducing greenhouse gas emissions [2], carbon-free energy sources have supplied a significant share of this additional demand. Nevertheless, fossil fuel consumption has continued to increase. Long-term trends in electricity generation from fossil fuels indicate a slowdown in the growth of both coal and natural gas; however, they still account for the largest share of global energy generation. As a consequence, the increase in energy production has been accompanied by a rise in CO_2 emissions of more than 50% since 2000.

In the current geopolitical context, fossil fuels represent a problematic source of energy not only in terms of environmental sustainability, but also due to security and affordability issues. The most emblematic event highlighting the intrinsic link between energy trade and the current fragile international environment is the Russian invasion of Ukraine in 2022, when Russia sought to gain political leverage by reducing natural gas supplies, thereby exposing European consumers to higher energy prices. The period of energy market volatility that followed, saw an acceleration in the deployment of renewable energy sources and efforts to improve energy efficiency in several key markets. Despite this, energy autonomy remains a distant prospect. According to Eurostat data [3], the European Union still relies heavily on imported oil and gas as its main energy sources. The relevance of this issue has been further reinforced in recent times by the impacts of the conflict in the Middle East. The war that began in the region on 28 February 2026 severely affected oil and gas trade flows through the Strait of Hormuz, creating one of the most significant supply disruptions in the history of the global oil market.

In this context, the development and deployment of alternative energy sources are essential. In principle, variable renewable energy (VRE) sources such as wind and solar, can deliver low-carbon power and represent a key part of the energy transition. However, they are non-dispatchable and characterized by low power density. As a result, an electricity

system dominated by VREs would require large-scale energy storage to balance supply and demand, as well as significant expansion of transmission infrastructure to deliver electricity from geographically distributed generation sites to demand centers. This would entail increasing costs and system complexity. In this framework, interest in nuclear energy has been renewed, as it constitutes a clean and limitless energy source that could provide a valuable alternative to fossil fuels and complement to renewable energy sources. Nuclear power plants based on fission reaction are a well-established and mature technology, currently deployed in several countries, offering significant advantages in terms of energy security and emissions reduction. They already account for a substantial share of the global energy mix, and their role is expected to grow in the coming decades. At the same time, significant efforts are being made in the field of fusion energy research. Indeed, the possibility of development of commercial fusion power plants is expected to help meet the growing demand for clean electricity, thanks to its high power density, flexible siting, virtually unlimited fuel availability, and inherent safety [4].

The work presented in this thesis is developed within this context and is carried out in the framework of fusion research. Section 1.1 introduces the fundamental physics of nuclear fusion reactions, followed by a discussion of *Magnetic Confinement Fusion (MCF)* technology, its current state of advancement, and its main challenges in Section 1.2. Finally, Section 1.3 addresses the issue of *plasma-wall interaction (PWI)* and discusses the related physical processes in detail.

1.1. Principles of nuclear fusion

The matter that constitutes the universe is composed of atoms, whose mass is predominantly concentrated in a very small ($\sim \text{fm}$), dense region of space known as the nucleus. Atomic nuclei are composed of nucleons, namely protons, which carry positive charge, and neutrons, which are electrically neutral. The number of protons determines the chemical element, whereas nuclei sharing the same proton number but differing in neutron number are referred to as isotopes.

A fundamental aspect of nuclear physics is that the total mass of a nucleus is always smaller than the sum of the masses of its individual constituents. This difference, known as the *mass defect*, can be understood in light of the equivalence between mass and energy, established by *Albert Einstein* in 1905 [5], and expressed by the relation $E = mc^2$ for a system at rest. The missing mass corresponds to the binding energy that holds the nucleus

together. Accordingly, the total nuclear mass can be written as [6]:

$$M = Zm_p + Nm_n - \frac{|\epsilon_b|}{c^2} \quad (1.1)$$

where Z is the atomic number (i.e. the number of protons), N is the neutron number, m_p and m_n denote the proton and neutron masses, respectively, and ϵ_b is the binding energy. This principle underlies the possibility of extracting and utilizing energy directly from atomic nuclei through nuclear reactions.

When a nucleus A collides with one or more nuclei or subatomic particles B , producing nuclides C and D , the process is referred to as a nuclear reaction:

$$A + B \rightarrow C + D \quad (1.2)$$

In a nuclear reaction, it is useful to distinguish between an *entrance channel* and an *exit channel*, each characterized by a specific set of particles and associated physical quantities (energy, mass, momentum, charge, etc.). During the reaction, the fundamental conservation laws of physics apply, e.g. energy conservation. Therefore, the total energy in the entrance channel (E_i) must equal that in the exit channel (E_f):

$$E_i = K_i + M_i c^2 = K_f + M_f c^2 = E_f \quad (1.3)$$

where M_i and M_f are the total initial and final masses of the particles in the entrance and exit channels, respectively (including possible contributions from nuclear excitation energy), and K_i and K_f are the corresponding total kinetic energies. The difference between these latter quantities defines the Q -value, given by:

$$Q = K_f - K_i = (M_i - M_f)c^2 \quad (1.4)$$

A positive Q -value corresponds to an exothermic reaction, since the increase in kinetic energy of the products relative to the reactants, results in a net release of energy to the environment. From Equation 1.4, it follows that $Q > 0$ only if the total mass in the exit channel is smaller than in the entrance channel [7]. Using Equation 1.1 and assuming that the number and type of nucleons are conserved during the reaction, this condition can be expressed in terms of binding energies:

$$Q = (M_i - M_f)c^2 = |\epsilon_{b,f}| - |\epsilon_{b,i}| \quad (1.5)$$

This implies that reactions leading to an energy release-and therefore exploitable for energy production-require that the nuclei in the exit channel are more tightly bound than those in the entrance channel.

As shown in Figure 1.1, the average binding energy per nucleon lies around 8 MeV for most nuclei and reaches a maximum at $A \simeq 56$. Therefore, there are two distinct scenarios in which an increase in binding energy leads to the release of energy: the splitting of heavy nuclei into lighter ones closer to the maximum (*nuclear fission*), and the merging of light nuclei into heavier ones (*nuclear fusion*). Nuclear fission is currently employed for electricity generation in nuclear power plants, where a chain reaction is initiated by the absorption of a neutron by heavy nuclei such as ^{235}U or ^{239}Pu . This process leads to the splitting of the nucleus into lighter fragments and the emission of additional neutrons, which sustain the reaction. In contrast, no commercial nuclear fusion reactors are currently available, as the field is still under active research.

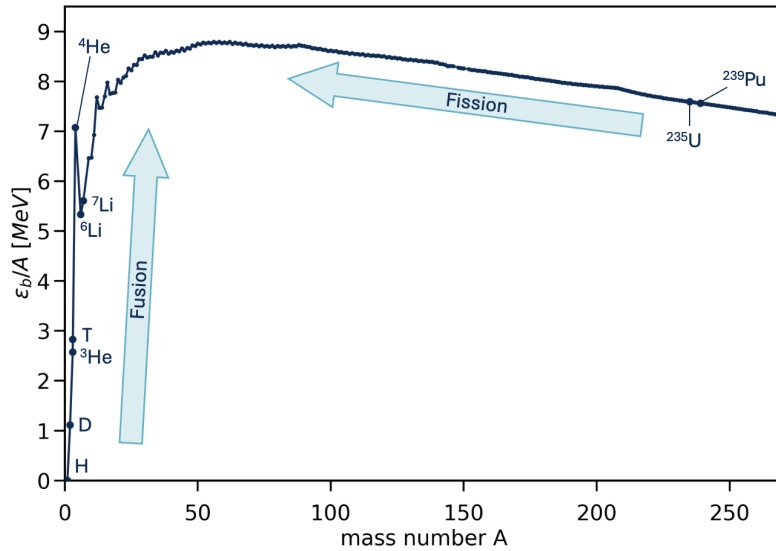


Figure 1.1: Average binding energy per nucleon as a function of the mass number A , based on data from [8], as recommended by IAEA (International Atomic Energy Agency) [9].

The choice of a suitable fusion reaction for energy production is a complex task, involving trade-offs among several parameters. A primary selection criterion is based on the Q -value and the reaction probability, quantified by the cross section σ . Nuclear fusion processes are strongly suppressed by the Coulomb repulsion between positively charged nuclei, which forms a barrier that must be overcome for the nuclei to approach sufficiently closely for the short-range nuclear force to prevail. Since the height of this barrier increases with the product of the nuclear charges, reactions involving nuclei with lower Z require

less stringent conditions to occur, making them preferred candidates for nuclear fusion applications. Some of the most relevant examples are reported below [10]:

$$\left\{ \begin{array}{ll} p + D \rightarrow {}^3\text{He} + \gamma & Q = 5.49 \text{ MeV} \\ D + D \rightarrow {}^4\text{He} + \gamma & Q = 23.85 \text{ MeV} \\ D + D \rightarrow {}^3\text{He} + n & Q = 3.27 \text{ MeV} \\ D + D \rightarrow T + p & Q = 4.03 \text{ MeV} \\ D + T \rightarrow {}^4\text{He} + n & Q = 17.59 \text{ MeV} \\ D + {}^3\text{He} \rightarrow {}^4\text{He} + p & Q = 18.35 \text{ MeV} \\ T + T \rightarrow {}^4\text{He} + 2n & Q = 11.33 \text{ MeV} \end{array} \right. \quad (1.6)$$

Among these, reactions producing ${}^4\text{He}$ (also known as α -particle) are particularly attractive, as this nucleus yields high Q -values due to its large binding energy, which results from its exceptional stability as a *double magic nucleus*¹.

The cross section σ depends on the relative kinetic energy of the colliding particles. In a classical framework, a particle can overcome the Coulomb barrier only if its kinetic energy exceeds the barrier height, implying the need for very high energies. In quantum mechanics, however, there is a non-zero probability for a particle to penetrate the barrier even at lower energies through the *tunneling effect*. As a result, the cross section is strongly influenced by the tunneling probability, which is well described by the *Gamow factor* $e^{-\sqrt{G_E}/\epsilon}$. Accordingly, the fusion cross section can be written as [7]:

$$\sigma(\epsilon) = \frac{1}{\epsilon} S(\epsilon) e^{-\sqrt{G_E}/\epsilon} \quad (1.7)$$

where ϵ is the center of mass energy of the reacting particles, $S(\epsilon)$ is the astrophysical S -factor, and G_E is the *Gamow energy*, proportional to the square of the charges of the interacting nuclei. In Figure 1.2a, cross sections for the most relevant reactions are shown.

Nevertheless, a key aspect is the enhancement of the reaction rate. For any binary reaction, this quantity can be expressed as:

$$R = n_1 n_2 \langle \sigma v \rangle \quad (1.8)$$

where n_1 and n_2 are the number density of the two reacting species and $\langle \sigma v \rangle$ is the

¹*Magic nuclei* are those in which either the proton number or the neutron number corresponds to a closed nuclear shell configuration. When both proton and neutron numbers are magic, the nucleus is referred to as double magic and exhibits enhanced stability.

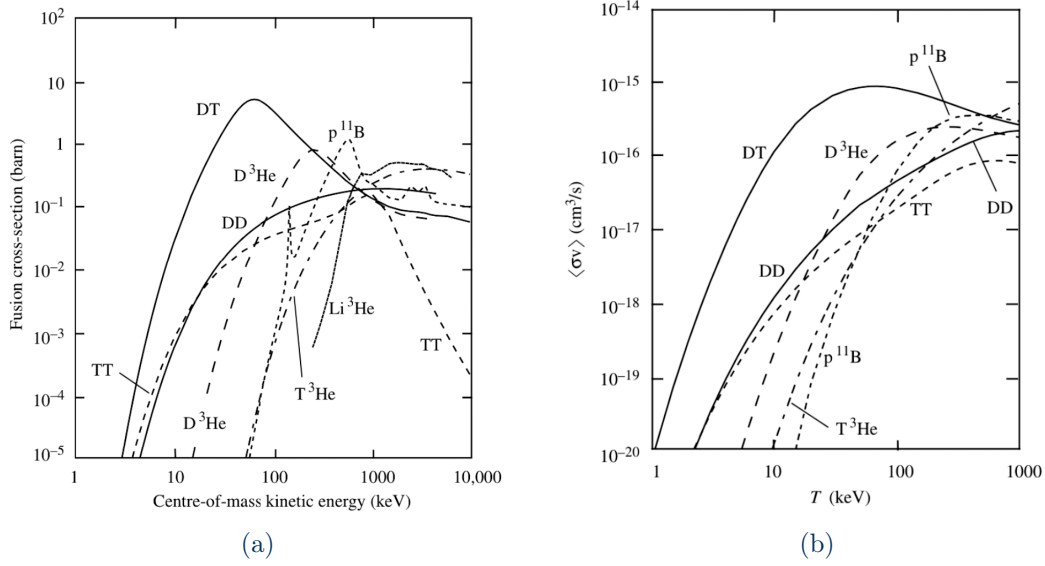


Figure 1.2: (a) Cross-sections (in barn) as a function of the center-of-mass energies of the reacting particles for various fusion reactions. (b) Reactivity averaged over a Maxwell-Boltzmann distribution as a function of temperature for the same fusion reactions [10].

reactivity. The latter is defined as the relative-velocity-weighted average of the cross section over a properly normalized velocity distribution function²:

$$\langle\sigma v\rangle = \int \sigma(v_r) v_r \hat{f}(v_r) dv_r \quad (1.9)$$

where v_r is the relative velocity. The cross section $\sigma(v_r)$ can be obtained directly from $\sigma(\epsilon)$ recalling that $\epsilon = \frac{1}{2}m^*v_r^2$, with $m^* = m_1m_2/(m_1 + m_2)$ being the reduced mass. If particles in a gas interact only through collisions, with no external forces or particle sources or sinks, the system reaches thermodynamic equilibrium after a time longer than the characteristic collisional time. In this regime, the system is described by a Maxwell-Boltzmann velocity distribution $f^{Max}(v)$:

$$f_a(v) = f^{Max}(v) = 4\pi n \left(\frac{m}{2\pi eT} \right)^{\frac{3}{2}} v^2 e^{-mv^2/2eT} \quad (1.10)$$

where the temperature is expressed in units of eV and defined as:

$$\frac{3}{2}enT = \frac{1}{2}m \int v^2 f(v) dv \quad (1.11)$$

²Here, $\hat{f}$ denotes the velocity distribution function normalized to the particle density, while f refers to the non-normalized distribution function.

Figure 1.2a shows the reactivity values obtained assuming a Maxwell-Boltzmann distribution for the most relevant fusion reactions. It can be observed that the highest values of $\langle\sigma v\rangle$, at relatively low energies, are achieved by the D-T reaction between the hydrogen isotopes deuterium (${}^2\text{H} = \text{D}$) and tritium (${}^3\text{H} = \text{T}$):



This process is currently considered the most promising, as it provides a high energy yield at the lowest required temperatures [11].

The enhancement of the fusion reaction rate in Equation 1.8 therefore requires not only a high reactivity, achieved at a specific - typically very high - temperature, but also high densities of the reacting charged particles. Such demanding conditions can be attained in *thermonuclear plasmas*. A plasma is a state of matter defined as a macroscopic, globally quasi-neutral system composed of charged particles, often accompanied by neutral species, in which the density of charged species is sufficiently high for collective behaviors and space-charge effects to arise, significantly influencing the system properties and electromagnetic behavior. The majority of research is directed towards the realization of nuclear fusion through thermonuclear plasmas, in which the fuel is in the plasma state and the high kinetic energies required to maximize the fusion probability are achieved by heating the system.

From a technological perspective, a self-sustaining fusion system requires heating the plasma to the temperatures necessary to initiate the reaction using an external heating source, and subsequently maintaining these conditions through the energy released by the fusion reactions themselves. To achieve net electricity production, an additional energy gain is required. The performance of a fusion reactor is commonly described by two dimensionless parameters:

$$Q = \frac{S_f}{S_{ext}} \quad Q_{eng} = \frac{P_{out}^{el}}{P_{in}^{el}} \quad (1.13)$$

Here, Q defines the plasma energy amplification efficiency, while Q_{eng} represents the overall plant efficiency, including all engineering efficiencies. S_f is the power produced by fusion reactions, S_{ext} is the external heating power given to the plasma and P_{out}^{el} and P_{in}^{el} are the electrical output and input power to the grid, respectively. It is defined as *breakeven* the condition in which the thermonuclear plasma is able to produce as much energy as it is required to heat it up, corresponding to $Q = 1$. Net energy production instead requires $Q_{eng} > 1$, implying that $Q > Q_{eng} > 1$. Power balance considerations are

therefore essential in identifying the operational requirements.

The energy released in a fusion reaction is converted into the kinetic energy of the reaction products and distributed among them inversely proportional to their masses. In the D-T reaction, the α particle carries approximately 3.5 MeV, while the neutron carries about 14.1 MeV. Being electrically charged, α particles remain confined and promptly deposit their energy in the plasma, providing a self-heating mechanism that sustains the temperature required to continue burning the fuel. Neutrons, being electrically neutral, are not confined and escape the plasma, carrying their energy beyond the first wall of the vessel, where it can, in principle, be converted into electricity via an appropriate thermodynamic cycle.

The global power balance for a steady-state thermonuclear plasma can thus be written in terms of source and loss terms. The sources include the external heating power (S_{ext}) and the power deposited by α particles (S_α), while the losses are mainly due to radiation (S_{rad}), such as Bremsstrahlung, and heat conduction losses (S_q):

$$\underbrace{S_{ext} + S_\alpha}_{\text{sources}} = \underbrace{S_{rad} + S_q}_{\text{losses}} \quad (1.14)$$

Each term appearing in Equation 1.14 can be expressed as a function of the plasma properties. Assuming a plasma with particle density n composed of equal amounts of D ($n_1 = n/2$) and T ($n_2 = n/2$) [11]:

$$S_\alpha = E_\alpha n_1 n_2 \langle \sigma v \rangle_{DT} = E_\alpha \frac{n^2}{4} \langle \sigma v \rangle_{DT} \quad (1.15)$$

$$S_{rad} = c_B Z_{eff}^2 n^2 T^{1/2} \quad (1.16)$$

$$S_q = \frac{3nT}{\tau_E} \quad (1.17)$$

Here, E_α is the kinetic energy carried by the α particle produced in a single fusion event, c_B is a constant, Z_{eff} is the *effective ion charge* and τ_E represents the conduction energy confinement time.

In the ideal case of negligible heat losses, a self-sustaining plasma, requiring no external power input ($Q \rightarrow \infty$), is obtained when $S_\alpha \geq S_{rad}$. This condition is satisfied only for temperatures exceeding the *ideal ignition temperature*, defined by the equality condition

$S_\alpha = S_{rad}$. By combining Equations 1.15 and 1.16, one obtains:

$$T_{id} = \left(\frac{\langle \sigma v \rangle_{DT} E_\alpha}{4 c_B} \right)^2 \quad (1.18)$$

This temperature depends only on the properties of the considered reaction. For the D-T reaction, $T_{id} = 4.4 \text{ keV}$, which is relatively low compared to other candidate fusion reactions, such as D-D, for which $T_{id} = 32 \text{ keV}$. This further highlights the advantage of D-T fuel for fusion applications.

The *ignition condition* represents a more realistic power balance situation, in which, at steady state, the alpha heating power balances both Bremsstrahlung and thermal conduction losses, without the need for external power input. Combining Equations 1.15, 1.16 and 1.17, the condition $S_\alpha \geq S_{rad} + S_q$ can be expressed as:

$$n\tau_E \geq \frac{12T}{\langle \sigma v \rangle E_\alpha - 4c_B T^{1/2}} \quad (1.19)$$

The quantity $n\tau_E$ is known as the *Lawson parameters*, and for D-T it reaches a minimum at $T \simeq 15 \text{ keV}$ ($\sim 1.74 \cdot 10^8 \text{ K}$). This temperature defines the least stringent condition for ignition which is commonly referred to as the *Lawson criterion* [12]:

$$n\tau_E \geq 2 \cdot 10^{14} \text{ s/cm}^3 \quad (1.20)$$

This condition can be satisfied under different operating regimes, depending on the relative values of n and τ_E . Two main approaches to plasma confinement have been investigated so far.

The first is the *Inertial Confinement Fusion (ICF)*, characterized by high densities n ($\sim 10^{23} - 10^{25} \text{ cm}^{-3}$) and short τ_E ($\sim \text{ns}$). The process is characterized by a fast dynamics and does not reach a steady state. A high-energy (MJ), nanosecond pulsed laser is used to irradiate a spherical fuel pellet. The interaction is mediated by an *ablator* layer, which is rapidly brought to a plasma state. The resulting ablation pressure generates a shock wave that compresses the inner fuel. As the density increases, the kinetic energy of the shock wave is converted into thermal energy at the center, forming a *hot spot* where fusion conditions are achieved. Several technological challenges are associated with ICF, including pellet fabrication, symmetry and efficiency of laser coupling, and optimization of the ablation process. The most advanced ICF facility is the *National Ignition Facility (NIF)* at Lawrence Livermore National Laboratory (LLNL) [13]. In December 2022, NIF achieved a major milestone by exceeding breakeven for the first time in a laboratory

experiment: an indirect-drive implosion produced 3.1 MJ of fusion energy from 2.05 MJ of laser input ($Q \geq 1.5$)³ [14].

The second approach is *Magnetic Confinement Fusion (MCF)*, which operates at lower densities n ($\sim 10^{14} - 15 \text{ cm}^{-3}$) and longer confinement times τ_E ($\sim \text{s}$). The present work focuses on this approach, which is described in more detail in the following Section 1.2.

Before that, a fundamental question arises: what is meant by *plasma confinement* and why is it so relevant? An unbounded plasma in vacuum, not subjected to any external electromagnetic field, expands while maintaining charge neutrality through *ambipolar diffusion*. Indeed, as a consequence of the *virial theorem*, a plasma cannot remain confined within a finite region of space solely by its self-generated electromagnetic field, and therefore requires the presence of an external field [15]. This implies that, if a plasma is left unbounded inside a vessel, it will freely expand until it reaches the walls, which act as both particle and energy sinks. From the perspective of fusion technology, this corresponds to significant thermal conduction losses, S_q , which act against the achievement of a power balance condition. The energy confinement time, τ_E , is in fact constrained, together with the plasma density n , by the Lawson criterion. In ICF, the target is compressed to extremely high densities, allowing the Lawson criterion to be satisfied for very short confinement times, short enough for the plasma to be confined by its own inertia. In MCF, on the other hand, the relatively low densities require much longer confinement times, which must therefore be achieved through the application of appropriately designed external magnetic fields.

1.2. Magnetic confinement fusion

In magnetic confinement fusion, longer energy and particle confinement times can be achieved, allowing for a possible steady-state operating condition, which is particularly favorable for energy conversion purposes in the perspective of future power plant design. For this reason, MCF is considered particularly promising, even though breakeven has not yet been achieved. The most significant result to date has been obtained by the Joint European Torus (JET) in Culham, Oxfordshire, in 1997. There, the first experiment using a 50-50 mixture of tritium and deuterium was carried out, setting a world record for magnetic fusion with an output power of 16 MW from an input heating power of 24 MW, corresponding to $Q = 0.67$ [16].

Figure 1.3 shows the current status and future program for fusion research within the

³This value is obtained by adopting a slightly different definition of Q , where S_{ext} denotes the laser energy instead of the power effectively absorbed by the plasma.

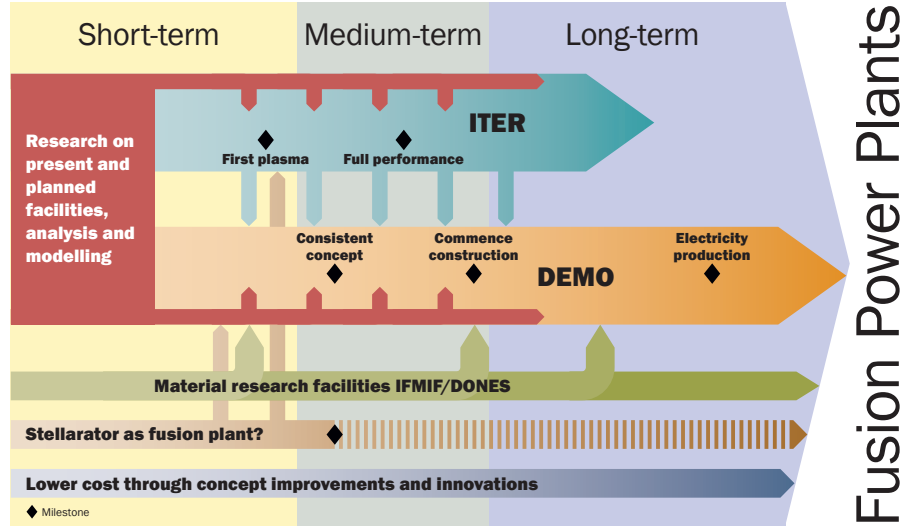


Figure 1.3: European research road-map for fusion energy realization [17].

European framework. The leading project is *ITER* (“The Way” in Latin) [19], the world’s largest and most advanced fusion experiment, currently under construction in southern France within an international collaboration involving China, Europe, India, Japan, Korea, Russia, and the United States. Besides being an outstanding example of international cooperation for peaceful purposes, *ITER* is expected to be the first magnetic confinement device to produce a net surplus of thermal fusion energy, with the goal of achieving $Q = 10$. *ITER* is intended to pave the way for the construction of *DEMO* (*Demonstration Power Plant*) [17], which is designed to be the first actual fusion power plant, reaching $Q_{eng} > 1$ and actively converting fusion energy into electrical energy.

The design of a complete fusion power plant is extremely complex, as it must address several technological challenges. A simplified scheme of the main components of a future MCF power plant is shown in Figure 1.4. The D-T plasma, where fusion reactions occur, is located at the core of the reactor. Neutrons escape the plasma, carrying about 4/5 of the released energy. A low- Z *blanket* surrounds the core, where neutrons transfer their kinetic energy through multiple collisions, thereby heating the blanket material. A cooling system embedded within the blanket removes this heat and feeds a thermodynamic cycle for electricity generation. An appropriate choice of blanket materials can also help address one of the main drawbacks of the D-T reaction: the limited availability of tritium. Tritium is an unstable isotope that undergoes β^- decay into ${}^3\text{He}$ with a half-life of 12.32

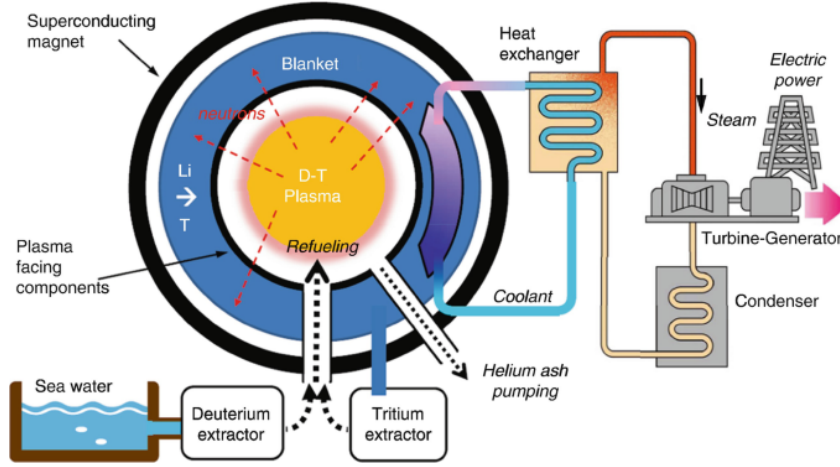
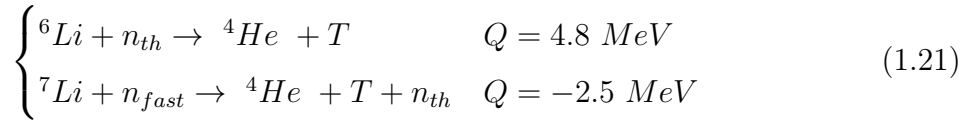


Figure 1.4: Schematic representation of a nuclear fusion power plant, from [18].

years, making large-scale storage difficult. Among low- Z materials, lithium plays a key role. Natural lithium consists of ${}^6\text{Li}$ (7.5%) and ${}^7\text{Li}$ (92.5%). Both isotopes can absorb neutrons and produce tritium through the following reactions:



This configuration is known as a *breeding blanket* and is capable of ensuring a self-sustaining supply of tritium for the fusion reaction.

To better understand the complexity and the main challenges of MCF, an overview of the fundamental principles underlying magnetic plasma confinement is first provided in Subsection 1.2.1. This is followed by a discussion of the main types of magnetic fusion devices in Subsection 1.2.2, and by an introduction to one of the key research challenges of magnetic confinement fusion, namely plasma-facing components, in Subsection 1.2.3.

1.2.1. Physics of magnetic confinement

To understand how a magnetic field can be used to confine a plasma, it is necessary to introduce some basic concepts of charged particle dynamics in magnetic fields, commonly referred to as *orbit theory*.

The simplest case is that of a constant and uniform magnetic field. In this situation, a charged particle follows a helical trajectory around a *magnetic field line*⁴, as shown in

⁴Field lines are imaginary directed curves that are everywhere tangent to the vector field. They describe the topological structure of the magnetic field and provide the basis for defining an intrinsic (or Frenet) frame.

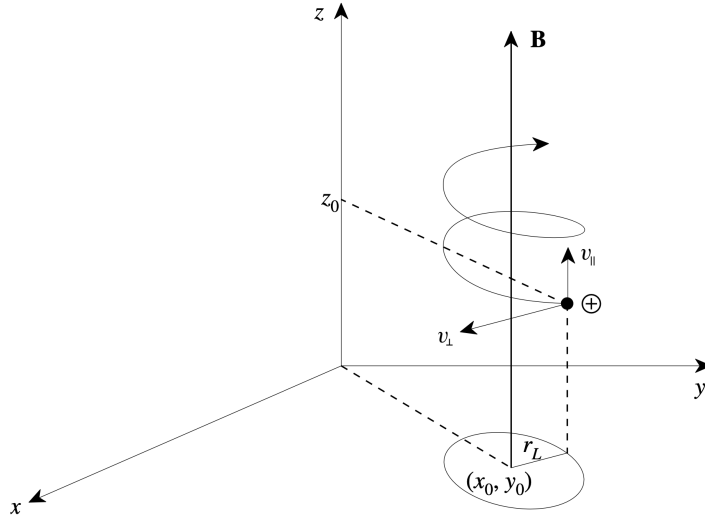


Figure 1.5: Orbit of a positively charged particle in a uniform magnetic field, from [20].

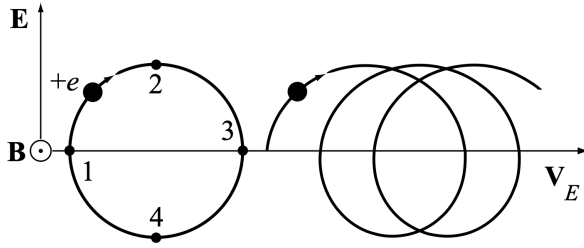


Figure 1.6: $\vec{E} \times \vec{B}$ drift of a positive charge, from [11].

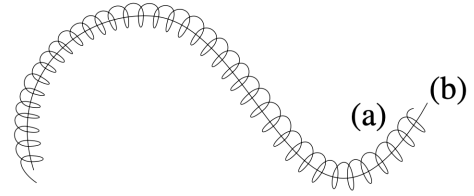


Figure 1.7: Charged particle motion in a non-uniform $\vec{B}$, showing (a) exact and (b) guiding-center trajectories, from [20].

Figure 1.5. The projection of the motion onto the plane orthogonal to the magnetic field is a circular trajectory, whose radius and frequency are known as the *Larmor radius* ρ_L and the *gyro-frequency* Ω_q , respectively⁵:

$$\Omega_q = \frac{qB}{mc} \quad \rho_L = \frac{v_\perp}{\Omega_q} \quad (1.22)$$

where q is the particle charge (its sign determining the sense of rotation), B is the magnetic field strength, m is the particle mass, and $v_\perp$ is the component of the velocity orthogonal to the magnetic field. The center of this circular motion, referred to as the *guiding center*, moves with constant velocity parallel to $\vec{B}$ [11]. In this framework, the average motion of the particle in the direction orthogonal to $\vec{B}$ is strongly suppressed.

⁵Only in this section *Gaussian metric system* is adopted for the expression of electromagnetic quantities.

In most situations, an external force $\vec{F}$ acts on the particle in addition to the magnetic field. The particle still undergoes a gyro-motion around its guiding center, but the latter's trajectory is modified by the presence of $\vec{F}$. Along the direction parallel to the magnetic field, the guiding center experiences a uniform acceleration determined by the parallel component of the force. The perpendicular component of the force, instead, induces a drift in the direction orthogonal to both the force and the magnetic field. The resulting *drift velocity* $v_{\perp,D}$ is given by [11]:

$$\vec{v}_{\perp,D} = \frac{c}{q} \frac{\vec{F}_{\perp} \times \vec{B}}{B^2} \quad (1.23)$$

In Figure 1.6 the particular case of the drift generated by an electric field $\vec{E}$ is reported, for which the drift velocity becomes

$$\vec{v}_{\perp,E} = c \frac{\vec{E}_{\perp} \times \vec{B}}{B^2} \quad (1.24)$$

A more realistic situation involves a non-uniform and, eventually, not-constant magnetic field. If $\vec{B}$ varies sufficiently slowly in both space and time, the particle motion can still be described, to zeroth-order, as a gyro-motion determined by the local magnetic field properties, while the guiding center moves along magnetic field lines. This approximation is known as the *guiding center approximation*, and is schematically depicted in Figure 1.7. Starting from this zeroth-order description, higher-order corrections can be introduced using a perturbative approach. The resulting particle dynamics includes several drift motions arising from different forces and effects. Among these, is worth mentioning at least the *grad-B drift* which originates from spatial variations of the magnetic field strength [11]:

$$\vec{v}_{\perp,\nabla B} = -\frac{c}{q} \mu \frac{\nabla B \times \vec{B}}{B^2} \quad (1.25)$$

where μ is the modulus of the *magnetic dipole moment* related to the gyro-motion of the charged particle.

At this point, it is useful to introduce a class of equilibrium magnetic field configurations that are particularly relevant for plasma confinement. A magnetic field is said to be static, if it satisfies the following equations:

$$\nabla \cdot \vec{B} = 0 \quad (1.26)$$

$$\nabla \times \vec{B} = \frac{4\pi}{c} \vec{J} \quad (1.27)$$

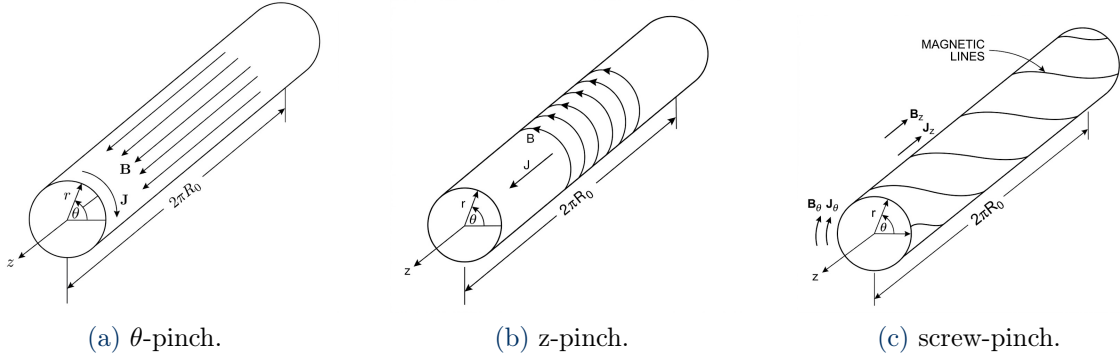


Figure 1.8: Cylindrically symmetric magnetic field equilibria configurations, from [15].

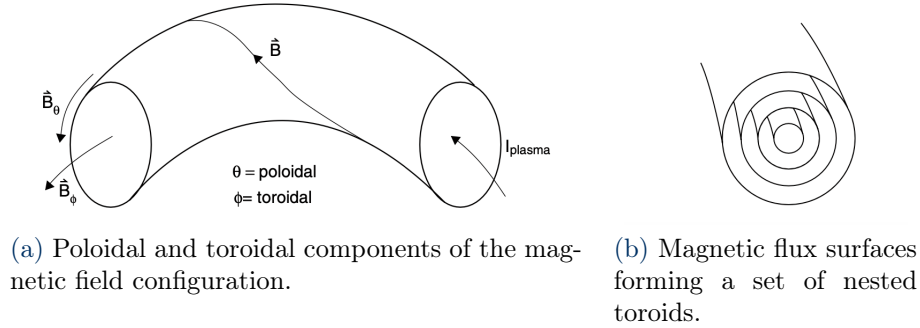


Figure 1.9: Toroidally symmetric magnetic field equilibrium configuration, from [22].

The magnetic field lines are ideally frozen inside the plasma [21], and accordingly to Equation 1.26 they have neither a beginning nor an end, and can therefore be either closed or infinitely extended (effectively closing at infinity). The set of points traced by a single infinitely long magnetic field line can ergodically cover a surface, defining a *magnetic surface*.

The simplest equilibrium configurations are one-dimensional, cylindrically symmetric systems that can be broadly classified into three types according to the properties of $\vec{B}$: *theta-pinch*, *z-pinch* or *screw-pinch*. In a *theta-pinch*, an external azimuthal current $\vec{J}_\theta$ generates an axial magnetic field $\vec{B}_z$ (1.8a). In a *z-pinch*, a current $\vec{J}_z$ is driven through the plasma, producing an azimuthal magnetic field $\vec{B}_\theta$ (1.8b). The *screw-pinch* combines these two configurations, resulting in magnetic field lines with both axial and azimuthal components (1.8c). Although these configurations can provide radial confinement, they fail to ensure axial confinement and are often characterized by poor stability. In particular, since the magnetic field lines are open-ended, they eventually intersect material boundaries, leading to significant end losses [15]. For this reason, such configurations are not suitable for fusion applications.

A natural improvement is obtained by bending the cylindrical system into a toroidal geometry. In this case, the magnetic field consists of two components: the *toroidal* component B_ϕ and the *poloidal* component B_θ .

$$\vec{B} = B_\phi \vec{e}_\phi + B_\theta \vec{e}_\theta \quad (1.28)$$

The resulting total magnetic field has a helical structure. The field lines are infinitely long and, in general, do not close on themselves but instead cover a magnetic surface ergodically (Figure 1.9a). The collection of these magnetic surfaces forms a set of nested toroidal surfaces, as shown in Figure 1.9b [22].

The achievement of toroidal equilibrium in magnetically confined plasmas requires satisfying both the radial force balance and the balance of the *toroidal forces*, which arise from the toroidal geometry itself. In the case of a purely toroidal magnetic field, the component B_ϕ exhibits a $1/R$ dependence (as follows from Equation 1.27), giving rise to a vertical *grad-B* drift. Since the drift direction depends on the sign of the particles charge, a separation of positive and negative species develops, leading to the formation of an electric field. The resulting $\vec{E} \times \vec{B}$ drift drives the plasma radially outward, thereby preventing equilibrium. Conversely, in a purely poloidal field configuration, forces such as the *hoop force* and the *tire tube force* tend to expand the plasma outward. Although these latter effects can, in principle, be compensated by a perfectly conducting shell or by external vertical field coils, such configurations are intrinsically unstable and prone to disruptions. As a result, a fundamental trade-off arises: systems dominated by poloidal fields exhibit better equilibrium properties but poor stability, whereas those dominated by toroidal fields are more stable but face significant equilibrium challenges. Modern magnetic confinement schemes aim to reconcile these opposing features by combining both field components to achieve a satisfactory compromise between equilibrium and stability [15].

1.2.2. Magnetic confinement devices: Tokamak and Stellarators

The toroidal magnetic confinement configuration is currently implemented in two main types of devices: *tokamaks* and *stellarators*.

The word "tokamak" is a Russian acronym for "**t**oroidál'naya **k**ámara s **m**agnítnymi **k**atúshkami", meaning "toroidal chamber with magnetic coils". The concept was originally developed in the USSR in the mid-1950s, based on the proposal of the scientists A. Sakharov and I. Tamm [24]. The first small-scale devices were relatively simple and lacked advanced control systems, but they nevertheless demonstrated that high-temperature plasmas could be produced and that energy confinement was achievable. In 1958, the

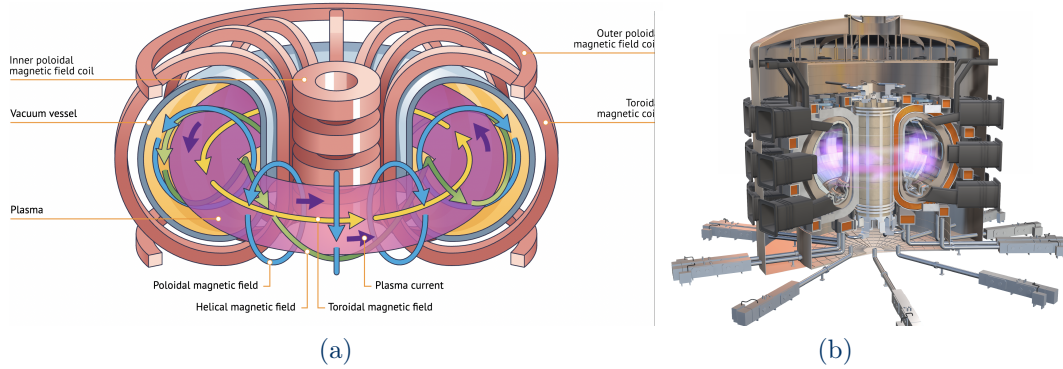


Figure 1.10: Tokamak fusion reactor: (a) schematic representation of the magnetic field configuration and coil system; (b) perspective view of the ITER reactor, from [23].

first fully operational tokamak began experiments, confirming the suitability of the tokamak concept for plasma confinement. Experimental progress continued steadily until 1968, when the T-3 tokamak achieved plasma temperatures and confinement times that had never been attained before [25]. From that point onward, the tokamak configuration became the dominant approach in fusion research, and such devices were rapidly developed worldwide. In current fusion research, this remains the leading approach, with both ITER and DEMO being tokamak-based reactors. The ITER project will be the world's largest tokamak, approximately twice the size of the largest machine currently in operation and featuring a plasma chamber volume about ten times greater [19].

Tokamaks implement a toroidal magnetic field configuration in two dimensions, exploiting toroidal symmetry. The toroidal magnetic field component is the dominant one and ensures the primary stability properties of the plasma; it is generated by external *toroidal field coils* that wrap around the torus in the poloidal direction. The poloidal magnetic field, on the other hand, is generated by a toroidal plasma current induced by an external *ohmic transformer*. This current also provides ohmic heating contributing to sustain the plasma. In addition, *vertical field coils* are used to ensure toroidal force balance, while *shaping coils* allow control of the plasma cross-section and contribute to improved stability [11]. A key limitation of tokamaks is that the toroidal plasma current, which is induced by a transformer, restricts their operation to pulsed regimes rather than steady-state conditions.

The stellarator is an inherently three-dimensional configuration, best described as a helically symmetric system bent into a torus. It was first conceived by L. Spitzer in 1951 at Princeton University [26] and dominated fusion research throughout the 1950s, but lost prominence when experimental studies on tokamak systems demonstrated their su-

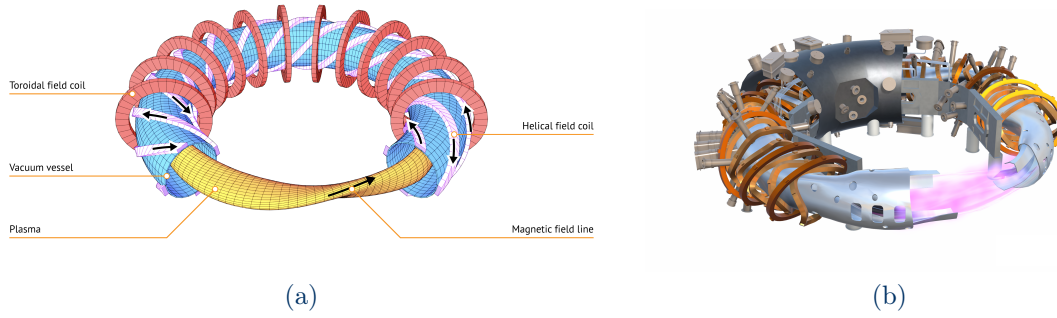


Figure 1.11: Stellarator fusion reactor: (a) schematic representation of the magnetic field configuration and coil system; (b) perspective view of a realistic reactor design, from [23].

terior confinement efficiency. In a stellarator, all components of the magnetic field are generated by external coils (*toroidal field coils* and *helical field coils*), so no ohmic or externally driven toroidal current is required. This makes the configuration intrinsically steady-state. Additionally, the absence of a significant net toroidal current substantially reduces the likelihood of major disruptions [11]. These features represent key advantages and are the main reasons why the stellarator concept was never completely abandoned; instead, it experienced a renewed interest in the 1990s, supported by advances in materials and manufacturing techniques as well as by private investments. On the other hand, stellarators present a major drawback compared with tokamaks: the coil system required to generate the magnetic field is significantly more complex from a technological standpoint. This leads to higher construction costs and potentially stricter limitations on the maximum achievable magnetic field [11].

1.2.3. Plasma-facing components: a major research challenge

The magnetic confinement of particles and energy in fusion-relevant plasmas is inherently imperfect. Particles move radially across magnetic flux surfaces, eventually reaching the wall of the vessel. Due to the high temperatures required to sustain fusion (see Section 1.1), if not properly controlled, this process can lead to intolerable particle and heat fluxes impinging on the so-called *first wall* of the tokamak. If the vacuum vessel were directly exposed to the plasma, its structure would be rapidly damaged, potentially developing burn spots and leaks. Moreover, such interactions would release significant amounts of impurities into the confined plasma, thereby degrading its performance [15].

The structural materials in direct contact with the plasma are referred to as *plasma-facing components (PFCs)* and constitute a crucial aspect in the design of a fusion reactor. The main technological challenge consists in exhausting the power from the core plasma with-

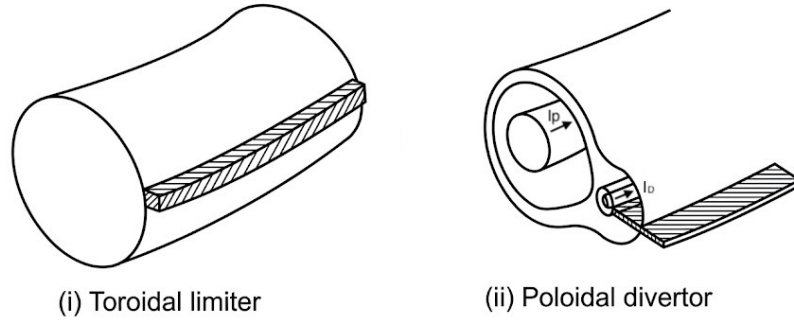


Figure 1.12: Tokamak plasma-facing configurations: the toroidal limiter and the poloidal divertor. Adapted from [22].

out causing intolerable damage to the first wall on one side, and without degrading plasma performance on the other [27]. Rather than allowing cross-field transport to distribute particle and power fluxes over the entire vessel surface, modern tokamaks employ a dedicated interface between the plasma and its surroundings. Two main types of such interfaces are currently used in tokamak experiments: the *mechanical limiter* and the *magnetic divertor* (Figure 1.12).

A mechanical limiter is a robust structure, typically made of tungsten, molybdenum, or graphite, and positioned just inside the vacuum chamber. To understand its working principle, it is necessary to recall that particle motion in a magnetically confined plasma, is strongly anisotropic, being predominantly directed along the magnetic field lines, i.e., $v_{\parallel} \gg v_{\perp}$. Therefore, when a particle crosses the edge of the plasma and enters the shadow region of the limiter, its large parallel velocity ensures that it will strike the limiter surface before diffusing further into the vacuum chamber [15]. In this way, the limiter acts as a particle sink, preventing particles from reaching the vessel walls. Consequently, plasma-surface interactions are localized on the limiter, which can be designed to withstand high heat and particle fluxes and can be more easily replaced than the entire vessel. In a toroidal geometry, limiters can be implemented in two configurations: the *poloidal limiter*, which protrudes into the plasma along a poloidal cross-section, and the *toroidal limiter*, which extends along the toroidal circumference.

The magnetic divertor concept, instead, consists in guiding a narrow layer of magnetic field lines - the outermost ones - away from the plasma confinement region. In a tokamak, a *poloidal divertor* configuration can be produced using external coils carrying a current I_D in the same direction as the toroidal plasma current I_p , as shown in Figure 1.12.

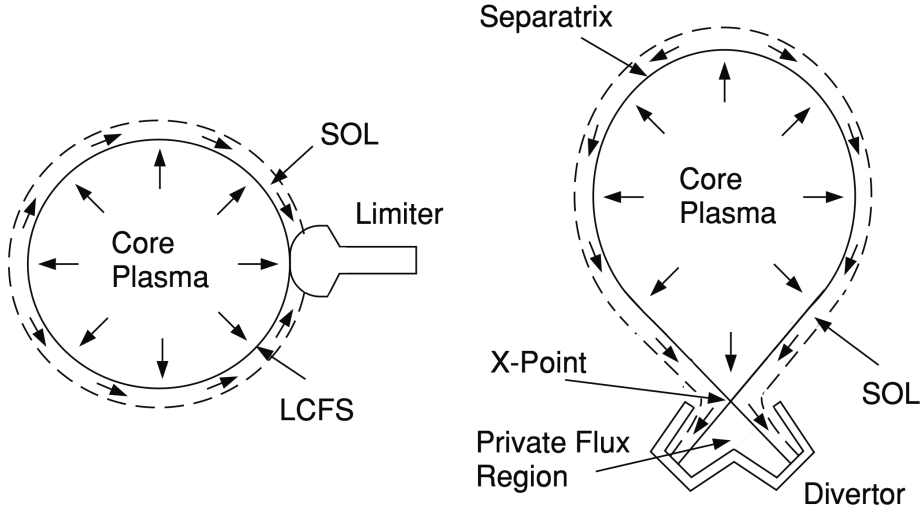


Figure 1.13: Scrape Of Layer (SOL) in limiter and divertor configurations, from [27].

In the poloidal plane, the resulting magnetic field lines form a characteristic figure-of-eight pattern. At a specific location between the current centers, the poloidal magnetic field vanishes, giving rise to a magnetic null point, known as the *X-point*. The magnetic flux surface passing through the X-point is called the *separatrix* [22]. Field lines just outside the separatrix are directed toward a remote region of the chamber, where they intersect robust collector plates, commonly referred to as *divertor targets*. Although toroidal divertor configurations also exist, the poloidal divertor is the standard choice in most tokamak designs.

Compared to limiter configurations, the divertor makes less efficient use of the magnetic volume, thereby increasing the overall cost, but offers several compensating advantages. Since the collector plates are located far from the main plasma, the heat flux can be sufficiently dissipated before reaching the walls, thereby reducing the intensity of particle and heat loads and increasing component lifetime. Additionally, since the edge of the core plasma does not directly contact solid surfaces, higher temperatures can be sustained, potentially leading to improved confinement [15]. This remote configuration also distances plasma-material interactions (PMI), limiting impurity transport back into the plasma. For all these reasons, the divertor configuration has become the preferred choice in modern designs.

In both configurations, it is possible to identify the *Last Closed Flux Surface (LCFS)*, defined as the outermost magnetic flux surface that does not intersect any material surface. The region inside the LCFS contains the confined plasma, whereas the region outside is known as the *scrape-off layer (SOL)*. A schematic representation of both limiter and

divertor configurations is shown in Figure 1.13.

In the divertor case, the LCFS coincides with the separatrix, and the region enclosed below the X-point is referred to as the *private plasma*, which is replenished solely by cross-field diffusion [22]. It is common to refer to the plasma region extending from just inside the separatrix to the first wall, as the *edge* or *boundary plasma*.

Overall, the management of plasma-surface interactions represents one of the major technological challenges in the development of magnetic confinement fusion reactors. Despite the adoption of limiter and divertor configurations to control particle and heat exhaust, plasma-facing components remain exposed to extreme thermal and particle loads. Their interaction with the edge plasma can cause material erosion, impurity release, and surface degradation, with important consequences for both reactor durability and plasma performance.

1.3. Plasma-wall interaction

The aforementioned challenges associated with *plasma-wall interaction (PWI)* make it clear that a deeper understanding of the underlying processes is required. This motivates the discussion of transport phenomena in edge plasmas of Subsection 1.3.1, where *cross-field diffusion* and the resulting imperfect confinement are addressed. Particular attention is then devoted to the plasma-surface interface in Subsection 1.3.2, with emphasis on the formation of the *electrostatic sheath* as the key mechanism governing their interaction. The analysis is further extended to the behavior of charged and neutral species inside a plasma, described in Subsection 1.3.3, focusing on the surface and volumetric reactions they undergo. Within this framework, *Linear Plasma Devices* are finally introduced in Subsection 1.3.4, as fundamental tools for investigating *plasma-material interaction (PMI)* in the context of fusion research.

1.3.1. Transport phenomena in edge plasma

The inherently imperfect nature of particle confinement, already introduced in Subsection 1.2.3, is here investigated and physically motivated in greater detail. According to the theoretical description of single-particle motion in a magnetic field, presented in Subsection 1.2.1, a charged particle in a stationary tokamak-like configuration remains confined to a given magnetic flux surface and, in principle, cannot migrate across magnetic surfaces. Therefore, the radial transport of particles may appear inconsistent with orbit theory.

In reality, single-particle dynamics alone is insufficient to describe a phenomenon arising in a many-particle system, where particles are not isolated but continuously interact with one another. Collisions and collective effects give rise to transport processes that can, at first approximation, be described as diffusion phenomena. The diffusion process may be interpreted in terms of a *random walk* performed by the particles. Their otherwise nearly free motion along the magnetic field lines is restricted by collisions, while radial transport is enhanced. During collisions, particles undergo random displacements across the magnetic field, with a characteristic step length of the order of the gyro-radius. This length scale is typically much smaller than the mean free path between successive collisions, which instead characterizes the motion parallel to the magnetic field lines [27].

In this context, net particle fluxes arise from the presence of plasma inhomogeneities. Any real plasma exhibits density gradients, which drive diffusion toward regions of lower density and therefore tend to flatten the density profile [27]. The relation between the particle flux and the density gradient can be expressed through the *Fick's law*, introducing a *diffusion coefficient* (Equation 1.29). Similar considerations apply to heat transport: temperature gradients generate thermal fluxes and the *thermal conductivity* relates the heat flux to the temperature gradient (Equation 1.30).

$$\vec{\Gamma} = -\underline{\underline{D}} \cdot \nabla n \quad (1.29)$$

$$\vec{q} = -\underline{\underline{\chi}} \cdot \nabla T \quad (1.30)$$

Here $\vec{\Gamma}$ and $\vec{q}$ denote the particle and heat fluxes, respectively, while $\underline{\underline{D}}$ and $\underline{\underline{\chi}}$ are the particle and thermal diffusivity tensors, containing information on both the parallel ($D_{\parallel}$, $\chi_{\parallel}$) and perpendicular ($D_{\perp}$, $\chi_{\perp}$) transport coefficients.

In the classical picture, the cross-field particle diffusion coefficient can be derived using the random-walk model [27]:

$$D_{\perp}^{classical} \simeq \nu \rho_{L,e} = \nu \left(\frac{v_e}{\Omega_e} \right) \propto \frac{1}{B^2} \quad (1.31)$$

where ν is the collision frequency. In this framework, $D_{\perp}^{classical}$ exhibits a $1/B^2$ dependence. Such a strong reduction of transport with increasing magnetic field strength initially raised great optimism regarding the rapid achievement of controlled thermonuclear fusion, since this scaling suggested that improved confinement could be obtained simply by increasing B . However, experiments soon revealed the presence of an anomalously large diffusion, exceeding the classical prediction by approximately four orders of magnitude, namely

$$D_{\perp}^{experiment} \simeq 10^{3-4} D_{\perp}^{classical}.$$

To account for this discrepancy, Bohm proposed a semi-empirical expression for the anomalous diffusion coefficient, from which a $1/B$ dependence emerges [28]. Although originally introduced without a rigorous derivation, this scaling can be naturally associated with $\vec{E} \times \vec{B}$ drifts generated by fluctuating electric fields. Consequently, anomalous transport in the SOL is generally attributed to turbulence and fluctuations in the electric field, arising from convective phenomena such as *zonal flows* and coherent vortex structures commonly referred to as *blobs* [27].

Despite the considerable theoretical and computational progress achieved in plasma transport studies, reliable predictive models are still difficult to obtain [27]. As a consequence, transport coefficients are often treated as effective constant input parameters in simulations and engineering estimates.

1.3.2. Electrostatic sheath

The physical processes occurring in the region of contact between a plasma and a solid surface are crucial in the context of plasma-wall interaction.

In the bulk plasma, the particle fluxes arising from thermal motion are always balanced, thanks to the overall isotropy of the system, and the *quasi-neutrality* condition is satisfied. In fact, by definition, a plasma is a globally quasi-neutral system, in which the negative and positive charge densities are nearly equal throughout the volume ($n_e \simeq \sum_i n_i = n$); this property is referred to as quasi-neutrality.

When a solid surface is brought into contact with the plasma, it acts a particle sink [22]. As a consequence the particle fluxes to the wall are no longer balanced. In thermal equilibrium the mobility of the electron population is typically much higher than that of the ions, due to their much smaller mass and inertia. Therefore, the electron flux to the wall is considerably higher than the ion flux, leading to the build-up of a negative space charge on the solid surface. The resulting electric potential then acts to reduce the electron flux and enhance the ion flux toward the surface. This leads to the formation of a positive space-charge region in the plasma adjacent to the solid boundary, known as the *plasma sheath* or *electrostatic sheath*. This process continues until a steady state is reached in which the electron and ion fluxes balance and the net current to the surface vanishes. In essence, the plasma responds to the perturbation of quasi-neutrality by establishing a self-consistent electric field that restores *ambipolar flow*. In this steady state, the surface potential is known as the *floating potential* [20].

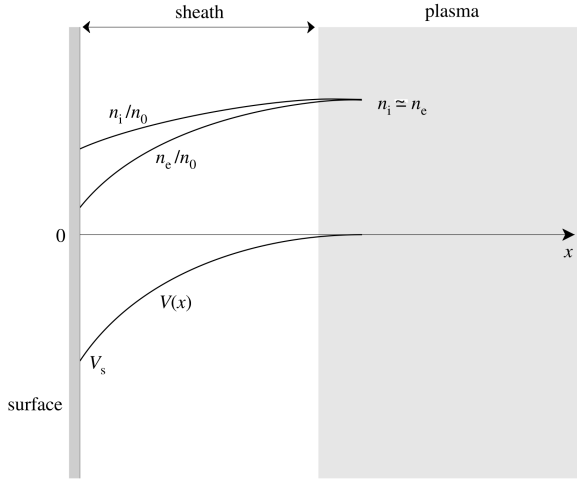


Figure 1.14: Formation of the plasma sheath near a material boundary, illustrating the spatial profiles of electric potential, electron density, and ion density, from [20].

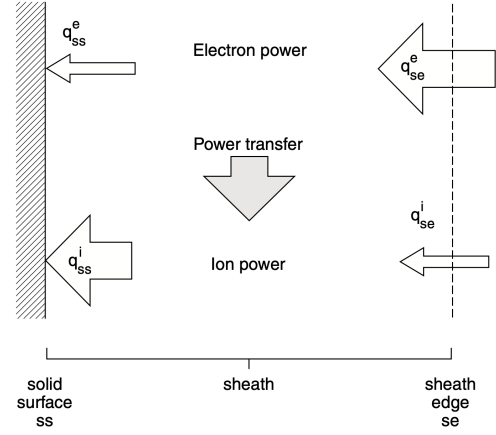


Figure 1.15: Electron and ion heat flux across the plasma sheath, from [22].

The sheath is a thin region of space in which plasma parameters and properties are strongly inhomogeneous, significantly deviating from those of the bulk plasma. It extends over a thickness of the order of the *Debye length*, which represents the characteristic scale of charge imbalance in a plasma, i.e. the length scale over which electrostatic screening occurs. For a plasma density n and an electron temperature T_e expressed in eV, the Debye length λ_D is given by [22]:

$$\lambda_D = \sqrt{\frac{\epsilon_0 T_e}{e n}} \quad (1.32)$$

The boundary between the sheath and the bulk plasma is not sharp, but rather a gradual transition. In fact, shielding within the sheath is imperfect, and a small electric field penetrates into the plasma, forming the so-called *pre-sheath* region. Here, the residual electric field drives ion motion from the upstream plasma, accelerating them toward the sheath. In 1949, Bohm showed that ions must enter the sheath with a velocity at least equal to the ion sound speed [28]. This requirement is known as the *Bohm sheath criterion*. From the plasma side, the ion velocity at the sheath edge cannot be greater than the sound speed c_s , therefore it should be exactly equal to c_s , commonly referred to as the *Bohm velocity*. In the case of a weakly coupled plasma, where $T_e \gg T_i$, the Bohm velocity is expressed as:

$$u_B \simeq \sqrt{\frac{e T_e}{m_i}} \quad (1.33)$$

Riemann extensively studied the Bohm criterion and, in 1991 [29], discussed its generalization for the case of non-negligible ion temperature T_i , yielding:

$$u_B = \sqrt{\frac{(T_e + \beta T_i)}{m_i}} \quad \beta = \begin{cases} 1 & \text{isothermal flow} \\ \frac{5}{3} & \text{adiabatic flow (with isotropic pressure)} \\ 3 & \text{1D adiabatic flow} \end{cases} \quad (1.34)$$

Crossing the sheath, both electrons and ions are lost to the wall. Assuming that the sheath is sufficiently thin such that no volumetric sources or sinks of particles occur within it, the particle flux is conserved between the sheath edge and the wall, i.e. $\Gamma_{se} = \Gamma_w$. Therefore, denoting by n_{se} the plasma density at the sheath edge, the Bohm criterion ensures that the ion flux to the wall can be written as [22]:

$$\Gamma_w^i = \Gamma_{se}^i = n_{se} u_B \quad (1.35)$$

Ambipolar transport requires equal ion and electron fluxes at the wall, therefore $\Gamma_w^e = \Gamma_w^i$. The electron flux can be expressed using the one-way particle flux density for a Maxwellian velocity distribution combined with the Boltzmann relation:

$$\Gamma_w^e = \frac{1}{4} n_w \bar{c}_e = \frac{1}{4} n_{se} e^{V_w/T_e} \bar{c}_e \quad (1.36)$$

where n_w and V_w are the electron density and the potential at the wall, respectively, and $\bar{c}_e = (8eT_e/\pi m_e)^{1/2}$ is the average electron thermal speed [22].

The potential drop that spontaneously develops between the plasma and a solid surface, V_{sf} , coincides with V_w when no external bias is applied. Combining Equations 1.35 and 1.36, the following expression for the floating potential is obtained:

$$\frac{V_{sf}}{T_e} = \frac{1}{2} \ln \left(2\pi \frac{m_e}{m_i} \left(1 + \frac{T_i}{T_e} \right) \right) \quad (1.37)$$

This expression typically yields values of the order of $V_{sf} \sim -3 T_e$. When an external bias is applied to the solid surface, the resulting change in the wall potential is entirely accommodated by the sheath, which continues to provide nearly perfect Debye shielding and thus maintains the plasma potential essentially unchanged. In this situation, the potential drop across the sheath must be corrected to include the additional applied contribution [22].

The sheath constitutes not only a particle sink but also an energy sink for the plasma. At

the sheath-solid interface, the power carried by the electrons is given by the forward-going heat flux density for a Maxwellian distribution [22]:

$$q_{ss}^e = 2T_e \Gamma_{ss} = 2T_e \Gamma_{se} \quad (1.38)$$

Nevertheless, this flux is not equal to the one at the sheath edge, which is larger. In fact, throughout the sheath, the generated electric field accelerates ions while slowing down electrons. This results in a net transfer of energy from the electrons to the ions, producing a cooling effect on the entire electron population of the plasma rather than a localized temperature drop within the sheath itself. The heat flux across the sheath is therefore conserved only when considering the combined ion and electron contributions, and not the two populations separately, as shown in Figure 1.15.

Ion acceleration actually begins in the pre-sheath region. Therefore, the total power loss experienced by the electron population through the sheath can be written as [22]:

$$q_{se}^e = (2T_e + |V_{sf}| + |V_{pre-sheath}|) \Gamma_{se} \quad (1.39)$$

where the pre-sheath potential drop is typically of the order of $|V_{pre-sheath}| \sim T_e/2$. For the ions, it can be shown that the heat flux at the sheath edge is [22]:

$$q_{se}^i = 2T_i \Gamma_{se} \quad (1.40)$$

Introducing the *sheath heat transmission coefficient* γ , the total heat flux can be expressed as:

$$q_{ss} = q_{se} = q_{se}^i + q_{se}^e = \gamma T_e \Gamma_{se} \quad (1.41)$$

The heat transmission coefficient accounts for both the electron and ion contributions, and its value depends on the specific plasma conditions [22].

1.3.3. Physics of charged and neutral species: surface and volumetric reactions

A wide variety of particles and species can coexist inside a plasma, all interacting both with one another and with the surrounding materials. Two main categories can be identified: charged particles and neutral species. These are not independent, since numerous reactions can occur among them within the plasma volume, leading to the production or loss of particles. At the same time, interactions with surfaces and with the external

environment can significantly affect the plasma composition.

Neutrals constitute the plasma fuel, being ionized through collisions with energetic electrons (*electron-impact ionization*). Through their interaction with electrons, they can also undergo *elastic* and *inelastic scattering*, eventually leading to excitation of electronic or vibrational levels when molecules are involved. In molecular plasmas, electrons may also induce the *dissociation* of neutral molecules.

Ions interact with both neutrals and electrons, giving rise to a wide range of processes. With neutrals, in addition to elastic and inelastic scattering, a key mechanism is *charge exchange*, where the ion transfers its charge to a neutral particle. Collisions with electrons are typically more frequent and can lead to *recombination* processes, or to dissociation in the case of molecular ions. In some plasmas, negative ions are also present, formed mainly via *electron attachment* and lost through *detachment* or recombination.

Overall, plasma chemistry is highly complex and becomes increasingly rich as the number of species grows, especially in molecular plasmas. These processes introduce volumetric source and loss terms for each species, as well as energy exchange mechanisms within the plasma. For instance, ionization and excitation processes generally represent an energy loss channel for electrons, while elastic scattering processes mainly redistribute energy among particles. The resulting chemical equilibrium depends strongly on parameters such as pressure and the temperatures of the different species, determining which reactions dominate under given conditions.

In this context, the so-called *surface reactions* play a major role. These processes involve the interaction between the plasma and solid materials which, as discussed in Section 1.3.2, constitute a sink for charged particles. Ions reaching the wall may be back-scattered or implanted into the material and later released as thermal neutrals after some residence time. In all cases, ions recombine at the surface and are re-emitted as neutrals, a mechanism known as *recycling*. In addition, surfaces where electrons accumulate can also support surface recombination processes, producing weakly bound neutral species that tend to desorb back into the plasma [22].

During the initial phase of a discharge, most ions reaching the wall (excluding promptly back-scattered particles) are retained by the material, so the wall behaves as an effective particle sink. However, once saturation is reached, a dynamic equilibrium is established: ions and electrons are continuously lost to the wall while recombined neutrals are re-emitted. In this regime, the wall no longer acts as a net mass sink but rather as a sink of charge and a source of neutrals. Since these neutrals constitute the fuel, the plasma becomes effectively *self-refueling* [22].

In molecular plasmas, surface effects also include additional processes such as the recombination of atomic species into molecules, as well as *quenching* of vibrationally excited molecules, which release part of their internal energy upon interaction with the wall.

A particularly relevant process in the framework of plasma-wall interactions is the *sputtering*. It consists of the erosion of material from the plasma-facing surfaces, resulting in the release of impurities into the plasma. Sputtering is therefore a major concern both due to the damage it causes to plasma-facing components and because of the detrimental impact on plasma performance induced by eroded particles migrating into the confined region. In fact, impurities generally increase the radiative power losses of the plasma.

Two main types of sputtering can be distinguished: *physical sputtering* and *chemical sputtering*. Physical sputtering occurs when an energetic incident ion strikes a solid surface and transfers sufficient momentum to an atom of the lattice, causing its ejection from the material. Chemical sputtering, instead, arises in the presence of reactive species, which can form chemical bonds with surface atoms, leading to the formation of volatile compounds that subsequently desorb from the surface.

1.3.4. Role of Linear Plasma Devices in fusion research

The discussion on plasma-wall interactions underlines the need for a deeper understanding of plasma-material interaction (PMI) processes and for the qualification of candidate plasma-facing materials for future fusion reactors. In particular, phenomena such as material erosion, surface morphology modification, impurity migration and redeposition, fuel retention, and dust production are of primary importance, as they strongly affect both reactor performance and component lifetime [30].

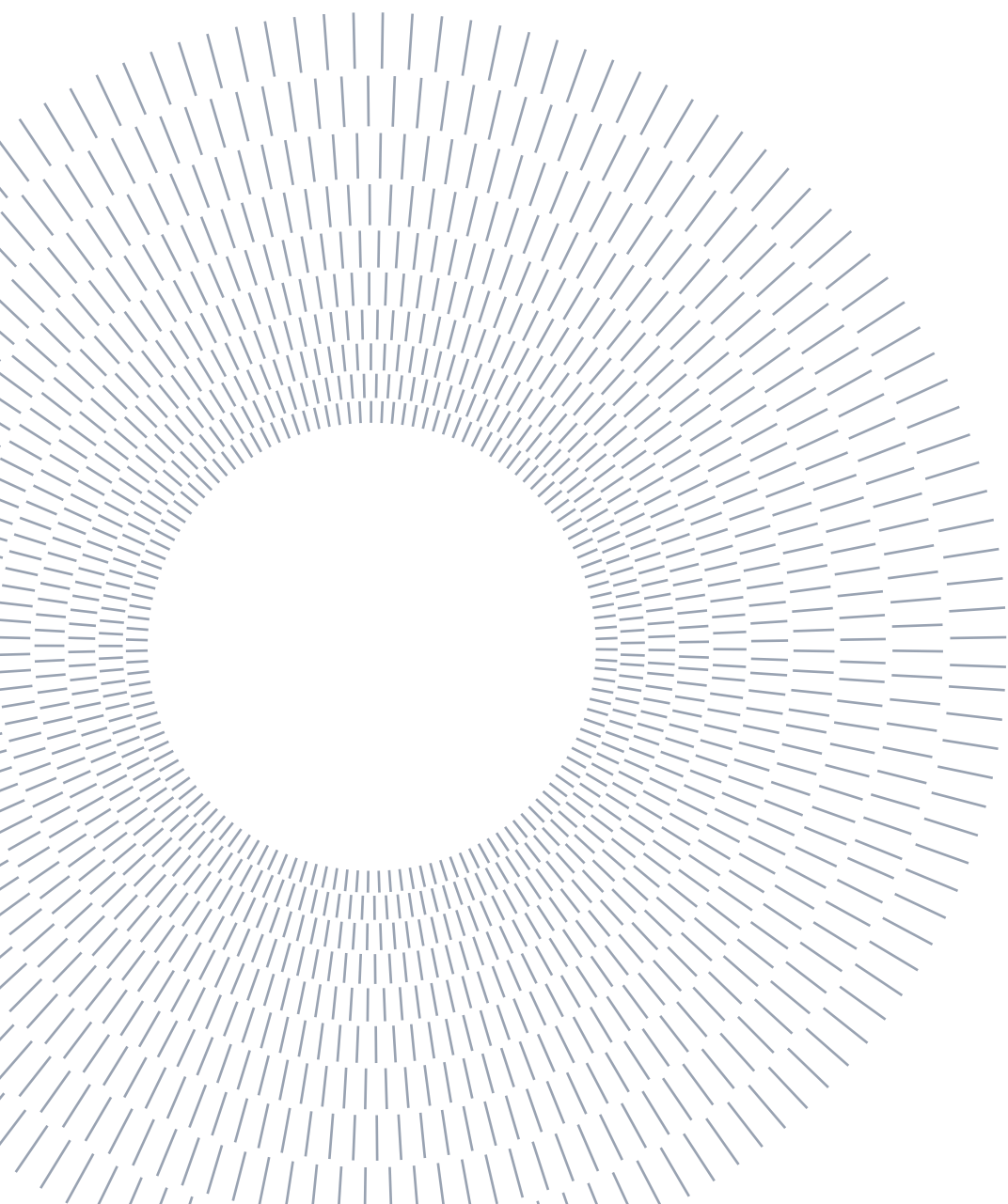
Some present-day tokamaks are already capable of reaching particle and heat fluxes at the divertor comparable to those expected in ITER, namely up to $\sim 10^{25}$ ions/m²s and 10 MW/m², respectively [31]. Nevertheless, sustaining steady-state operation for long pulse durations under these conditions remains beyond current capabilities [30]. Since ITER is designed to operate with discharge durations of about 1000 s, significantly larger fluences will be achieved compared to present-day devices. Consequently, several aspects of PWI are still not fully experimentally investigated, including ion fluxes and fluences at strike points, plasma-facing component temperatures, the behaviour of neutron-irradiated materials, and the evolving elemental composition of both plasma and wall materials [32].

Linear plasma devices (LPDs) provide a complementary approach to address these research gaps at moderate costs and with existing technologies. These devices can generate controllable particle fluxes under steady-state conditions for extended operation times,

reaching ion fluxes and fluences relevant to both first-wall and divertor scenarios foreseen in future tokamaks. As a result, they are particularly suitable for investigating material erosion, fuel recycling, impurity production, redeposition, and basic aspects of plasma detachment. [32].

The exploited magnetic configurations are typically one-dimensional and cylindrically symmetric, with a vacuum chamber surrounded by magnetic coils that generate an axial magnetic field through externally driven azimuthal currents.

Among the major LPD facilities used for plasma-material interaction studies are Dutch Institute for Fundamental Energy Research's Magnum-PSI in Eindhoven [33], the Material Plasma Exposure eXperiment (MPEX) at Oak Ridge National Laboratory [34], and PSI-2 at Forschungszentrum Jülich [35]. To these the Italian GyM [36] linear device can be added, which will be described in more detail in Chapter 4, as it constitutes the experimental reference for the modelling activities presented in this work.



2 | Theoretical and numerical models for edge plasma

Studying plasma dynamics frequently requires the use of theoretical physical models. Such models are mathematical representations of physical systems, built to capture their behavior while setting aside unnecessary complexity.

In plasma physics, various models can be employed to provide a self-consistent description of the plasma together with the electromagnetic field, each characterized by a different level of detail and approximation. Beginning from a first-principles description, successive levels of approximation can be introduced, with each step inevitably sacrificing some information in exchange for reduced complexity. As a result, each model proves more suitable in a specific context, depending on the application, the phenomenon of interest, and the relevant temporal and spatial scales. The ability to simplify the description of a system is not only essential for making it more tractable, but also because, when applied in the appropriate context, it can bring certain physical properties and phenomena into sharper focus. On the other hand, excessive simplification risks obscuring key dynamical effects, leading to an incomplete or inaccurate picture of plasma behavior. Choosing the right model for the right context is therefore of fundamental importance, underscoring the need for a thorough understanding of the available theoretical frameworks [11].

Figure 2.1 illustrates the hierarchy of the most relevant plasma models. The *ab initio* approach represents the first-principles description, carrying the highest level of information. It comprises a system of equations describing the dynamics of every individual particle, coupled with Maxwell's equations for the electromagnetic field. However, the sheer number of particles typically involved renders this model practically intractable.

The *kinetic model* represents the next level of simplification. Rather than tracking individual particles, it transitions from a microscopic to a macroscopic description. The

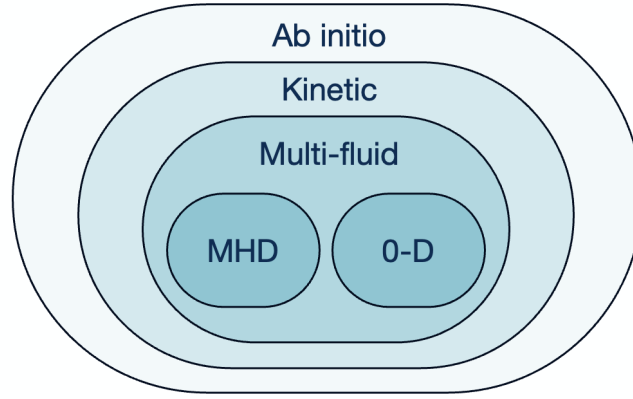


Figure 2.1: Schematic representation of the hierarchy of theoretical plasma models, spanning from first-principles *ab initio* approaches to reduced-order descriptions.

model describes the system dynamics within an *Eulerian*¹ framework, employing particle distribution functions defined in *phase space*, which depend on both spatial and velocity coordinates. The governing equations are derived and discussed in detail in Section 2.1.

The *multi-fluid model* represents a further step forward, where the plasma is described as a system composed of different interacting fluids, one for each species, coupled self-consistently to the electromagnetic field. The properties of each fluid are described through appropriate *macroscopic dynamical fields*. The derivation of the governing equations is discussed in detail in Section 2.2.

Starting from the multi-fluid model, different kinds of approximations can be introduced, leading to different plasma models. Figure 2.1 reports two possible approaches: the *magneto-hydrodynamics (MHD) model* and the *global (0D) models*.

In the MHD model, the plasma is treated as a single fluid. This approach is suitable in contexts where the separate dynamics of the different plasma species do not play a significant role. Since it is not directly relevant to the scope of this thesis, it will not be discussed further.

Global models, instead, constitute the main focus of this work. They are obtained by performing a spatial, and in some cases temporal, averaging of the multi-fluid equations, resulting in a point-like description of the plasma. Despite their simplicity, they provide estimates of species densities and temperatures at a very low computational cost. Their reduced complexity also enables the inclusion of detailed plasma chemistry, while allowing

¹A *Lagrangian* description follows the evolution of individual particles along their trajectories, whereas an *Eulerian* description considers fixed points in space and describes how the properties of the particle population vary at those locations.

the underlying physical mechanisms to emerge more clearly than in higher-fidelity models. The formulation and implementation of 0D models are extensively discussed in Section 2.3, together with a literature overview focused in particular on hydrogenic plasmas.

The presented theoretical models are hardly solvable analytically, even in their simplest forms. For this reason, they are typically approached numerically. Section 2.4 addresses the topic of numerical plasma modeling, with particular focus on the multi-fluid SOLPS-ITER code [37, 38]. Finally, Section 2.5 discusses the motivations behind this thesis and its main objectives.

2.1. Kinetic plasma model

In the kinetic model framework, the properties of plasma species are described in terms of macroscopic distribution functions, which provide the particle density in phase space². These distribution functions f are defined macroscopically as suitable ensemble averages of the microscopic distribution functions f_{micr} , which describe the plasma dynamics in an Eulerian first-principles framework. The averaging volume is chosen to be sufficiently large to contain a statistically significant number of particles, but sufficiently small to ensure that the resulting macroscopic distribution function f does not vary significantly over it. In this framework, microscopic quantities can always be expressed as the sum of their macroscopic counterparts and the corresponding microscopic fluctuations:

$$\begin{aligned} f &= \langle f_{micr} \rangle \\ f_{micr} &= f + \tilde{f} \end{aligned} \tag{2.1a}$$

Here, the brackets $\langle \dots \rangle$ denote the averaging operator, and $\tilde{f}$ represent the fluctuation of f_{micr} with respect to its mean value, satisfying the property $\langle \tilde{f} \rangle = 0$.

By introducing an evolution equation for the macroscopic distribution function, it becomes possible to describe the dynamics of the different species. Such equation can be derived by considering the variation in the number of particles within an infinitesimal six-dimensional volume element in phase space, $d^3x \, d^3v$. Variations in the particle content within such volume may arise in two ways: through the creation or destruction of particles due to collisions and reactions, or through an imbalance between incoming and outgoing fluxes in phase space - comprising both particle motion in configuration space and velocity changes under the action of external forces [39].

²Phase space is a six-dimensional space where both position and velocity are treated as independent variables

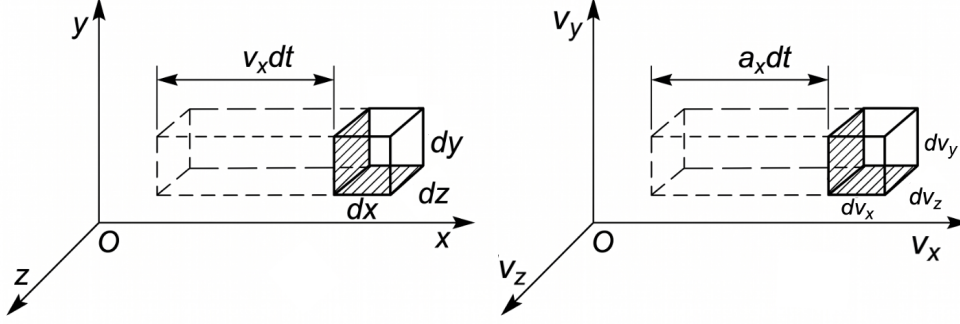


Figure 2.2: Particle flux balance in phase space, adapted from [39].

First of all, the balance of particle fluxes for the volume element d^3x (i.e. $dx dy dz$) along the x direction through the surface element $dy dz$ is considered. As shown in Figure 2.2, during the time interval dt , all the particles contained in the volume $v_x dt dy dz$ enter the volume d^3x . If f_a is the distribution function of the a -th species, then the number of incoming particles is given by $[f_a v_x]_x dt dy dz d^3v$. Analogously, the number of particles exiting the volume at position $x + dx$ is expressed as $[f_a v_x]_{x+dx} dt dy dz d^3v$. Therefore, the variation in the number of particles contained in the volume, associated with the difference between the incoming and outgoing fluxes in the x direction, is given by [39]:

$$\left[\frac{\partial f_a}{\partial t} \right]_x dt d^3x d^3v = ([f_a v_x]_x - [f_a v_x]_{x+dx}) dt dy dz d^3v = -\frac{\partial(f_a v_x)}{\partial x} dt d^3x d^3v \quad (2.2)$$

The same procedure can be repeated for the y and z spatial coordinates, yielding analogous contributions. Particles can also enter and exit the velocity-space volume d^3v (i.e. $dv_x dv_y dv_z$) because of variations in velocity generated by an acceleration $\vec{a}$ induced by a force $\vec{F}$. This term can be treated analogously to the previous one, recalling that in a plasma particles are subjected to the *Lorentz force*:

$$\vec{a} = \frac{q_a}{m_a} \left(\vec{E} + \vec{v} \times \vec{B} \right) \quad (2.3)$$

where q_a and m_a are the charge and the mass of the a -th species, respectively [39].

The collision term comprises two distinct types of interactions. The first type consists of short-range electromagnetic forces, which alter a particle's speed and trajectory but not its identity; as a result, these interactions do not produce exchange terms between different particle populations. The second type includes chemical and nuclear reactions, which typically introduce exchange contributions across different particle populations. Through-

out this discussion, the first contribution is denoted as $\left(\frac{\delta f_a}{\delta t}\right)_{coll}$, while the second will be represented by $S(\vec{x}, \vec{v})$ [22]. Given that these effects originate at the microscopic scale, they cannot be directly incorporated into the macroscopic kinetic framework without dedicated modeling assumptions. In fact, the collision term $\left(\frac{\delta f_a}{\delta t}\right)_{coll}$ inherently depends on second-order correlations of the fluctuations $\tilde{f}$. Describing the evolution of these second-order correlations, however, requires knowledge of third-order correlations, which in turn demand fourth-order ones, and so forth. The result is an infinite chain of mutually coupled equations. To render the problem solvable, this hierarchy must be truncated at some chosen order, which inevitably requires an approximation or *closure model*. Different approaches have been developed and investigated. The simplest one is the *Vlasov* closure, which neglects the collision term by setting it equal to zero. This approximation is valid only under the assumption of a *collisionless plasma*, a condition that is generally well satisfied in sufficiently hot and dilute plasmas.

Collecting all contributions together – the spatial flux terms, the velocity-space flux terms due to the Lorentz force, and the collisional source term – the evolution equation for the distribution function can be written as [39]:

$$\frac{\partial f_a}{\partial t} + \vec{v} \cdot \frac{\partial f_a}{\partial \vec{x}} + \frac{q_a}{m_a} \left(\vec{E} + \vec{v} \times \vec{B} \right) \cdot \frac{\partial f_a}{\partial \vec{v}} = \left(\frac{\delta f_a}{\delta t} \right)_{coll} + S(\vec{x}, \vec{v}) \quad (2.4)$$

This equation is called the *kinetic equation* or *Boltzmann equation*, and it can only be solved once the fields $\vec{E}$ and $\vec{B}$ are known. A self-consistent treatment therefore requires coupling the Boltzmann equation with Maxwell's equations. Hence, the complete set of equations constituting the kinetic model is given by:

$$\left\{ \begin{array}{l} \nabla \cdot \vec{E} = \frac{\rho_{ext} + \sum_a \rho_a}{\epsilon_0} \\ \nabla \cdot \vec{B} = 0 \\ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{B} = \mu_0 \left(\vec{J}_{ext} + \sum_a \vec{J}_a \right) + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} \\ \frac{\partial f_a}{\partial t} + \vec{v} \cdot \frac{\partial f_a}{\partial \vec{x}} + \frac{q_a}{m_a} \left(\vec{E} + \vec{v} \times \vec{B} \right) \cdot \frac{\partial f_a}{\partial \vec{v}} = \left(\frac{\delta f_a}{\delta t} \right)_{coll} + S(\vec{x}, \vec{v}) \end{array} \right. \quad (2.5)$$

$$\left\{ \begin{array}{l} \rho_a = q_a \int f_a d^3v \\ \vec{J}_a = q_a \int \vec{v} f_a d^3v \end{array} \right.$$

where ρ_a and $\vec{J}_a$ are the charge and current densities of the a -th species, respectively, while ρ_{ext} and $\vec{J}_{\text{ext}}$ are the external charge and current densities, respectively.

2.2. Multi-fluid plasma model

The multi-fluid model consists in a set of equations for the *moments* of the distribution function. These moments are obtained by averaging suitable functions of the particle velocity, denoted by ψ , over the velocity distribution function f_a [39].

$$\langle \psi(\vec{v}) \rangle_a = \frac{\int \psi f_a d^3v}{n_a} \quad (2.6)$$

where n_a represents the particle density of the a -th species and is defined as:

$$n_a(\vec{x}, t) = \int f_a d^3v \quad (2.7)$$

The function ψ may correspond to moments of different order. The most relevant cases are [15]:

$$\begin{cases} \psi = 1 & \text{zero - th order (particle)} \\ \psi = m_a \vec{v} & \text{first order (moment)} \\ \psi = \frac{1}{2} m_a v^2 & \text{second order (kinetic energy)} \end{cases} \quad (2.8)$$

This averaging procedure in phase space removes the dependence on the velocity coordinates, yielding a description of the plasma properties in terms of macroscopic dynamical fields defined in configuration space. As a consequence, a single velocity field $\vec{u}_a$ is associated with each plasma species, analogously to a fluid description:

$$\vec{u}_a(\vec{x}, t) = \frac{\int \vec{v} f_a d^3v}{n_a} \quad (2.9)$$

In this framework, each plasma species is treated as a separate fluid, while the plasma itself is regarded as an ensemble of coupled fluids [15].

The fluid velocity $\vec{u}_a$ represents the mean particle velocity, with respect to which a fluctuating velocity component, $\vec{v}'$, associated with random thermal motion, can be defined:

$$\vec{v}' = \vec{v} - \vec{u}_a \quad (2.10)$$

$$\langle \vec{v}' \rangle = 0 \quad (2.11)$$

The governing equations for the moments of the distribution function correspond to the fluid equations and are obtained by applying the averaging operator $\langle \psi(\vec{v}) \rangle_a$ to the kinetic equation [40]:

$$\frac{\partial}{\partial t} n_a \langle \psi \rangle_a + \nabla \cdot (n_a \langle \psi \vec{v} \rangle_a) - \frac{q_a}{m_a} n_a \left\langle \left(\vec{E} + \vec{v} \times \vec{B} \right) \cdot \frac{\partial \psi}{\partial \vec{v}} \right\rangle_a = n_a \langle C_a \psi \rangle_a \quad (2.12)$$

where, at this first stage of the derivation, the particle creation and destruction term due to reactions, $S(\vec{x}, \vec{v})$, is neglected, so that $C_a \equiv \left(\frac{\delta f_a}{\delta t} \right)_{coll}$. From this the fluid equations for each species can be derived [40, 41].

$$\text{Continuity equation:} \quad \frac{\partial n_a}{\partial t} + \nabla \cdot (n_a \vec{u}_a) = 0 \quad (2.13)$$

$$\begin{aligned} \text{Momentum balance equation:} \quad \frac{\partial}{\partial t} (n_a m_a \vec{u}_a) + \nabla \cdot (n_a m_a \vec{u}_a \vec{u}_a) = \\ = -\nabla \cdot \underline{\underline{P}}_a + q_a n_a \left(\vec{E} + \vec{u}_a \times \vec{B} \right) + \vec{R}_a \end{aligned} \quad (2.14)$$

$$\begin{aligned} \text{Energy balance equation:} \quad \frac{\partial}{\partial t} \left(\frac{3}{2} n_a T_a \right) + \nabla \cdot \left(\frac{3}{2} n_a T_a \vec{u}_a \right) = \\ = -\nabla \cdot \vec{q}_a - \underline{\underline{P}}_a : \nabla \cdot \vec{u}_a + Q_a \end{aligned} \quad (2.15)$$

The *total pressure tensor* $\underline{\underline{P}}_a$ can be considered as the sum of an *isotropic part* corresponding to the scalar plasma pressure, $p_a \underline{\underline{I}}$, and an *anisotropic part* $\underline{\underline{\Pi}}_a$ [15]:

$$\underline{\underline{P}}_a \equiv n_a m_a \langle \vec{v} \vec{v}' \rangle_a \quad (2.16)$$

$$\underline{\underline{P}}_a = p_a \underline{\underline{I}} + \underline{\underline{\Pi}}_a \quad (2.17)$$

The scalar pressure p_a is related to the mean energy associated with the disordered particle motion and is therefore connected to the plasma temperature [40]:

$$\frac{3}{2} n_a T_a = \int \frac{1}{2} m_a |\vec{v}|^2 f_a d^3 v \quad (2.18)$$

$$p_a = \frac{1}{3} m_a \int |\vec{v}|^2 f_a d^3 v = n_a T_a \quad (2.19)$$

The *conductive heat flux density* $\vec{q}_a$ describes the transport of thermal energy due to the

random particle motion and is defined as [15]:

$$\vec{q}_a = \frac{1}{2} m_a n_a \langle v'^2 \vec{v}'_a \rangle \quad (2.20)$$

Finally the two terms arising from collisions between unlike particles are the mean momentum transfer due to friction $\vec{R}_a$, and the generated heat Q_a [15].

$$\vec{R}_a = \int m_a \vec{v} C_{a,b} d^3 v \quad (2.21)$$

$$Q_a = \int \frac{1}{2} m_a v'^2 C_{a,b} d^3 v \quad (2.22)$$

Here $C_{a,b}$ is a quantity defined in phase space, which describes the variation per unit time of particles of kind a due to collision with particles of kind b . It can be shown that [40]:

$$\left\{ \begin{array}{l} \int C_{a,b} d^3 v_a = 0 \end{array} \right. \quad (2.23)$$

$$\left\{ \begin{array}{l} \int m_a \vec{v}_a C_{a,b} d^3 v_a = - \int m_b \vec{v}_b C_{b,a} d^3 v_b \end{array} \right. \quad (2.24)$$

$$\left\{ \begin{array}{l} \int \frac{1}{2} m_a v_a^2 C_{a,b} d^3 v_a = - \int \frac{1}{2} m_b v_b^2 C_{b,a} d^3 v_b \end{array} \right. \quad (2.25)$$

Equation 2.23 explains the absence of a collisional term in the continuity equation (2.13), since collisions conserve the total number of particles. Reintroducing particle generation and destruction due to reactions, which were originally neglected, gives rise to additional source terms on the right-hand side (RHS) of the fluid equations, given by

$$\int \psi S(\vec{x}, \vec{v}) d^3 v . \quad (2.26)$$

Any plasma model must be coupled self-consistently with the electromagnetic field, and the multi-fluid model is no exception. Consequently, Maxwell's equations must be solved together with the fluid equations, using suitably defined charge and current densities:

$$\rho_a = q_a n_a = q_a \int f_a d^3 v \quad (2.27)$$

$$\vec{J}_a = q_a \vec{v}_a = q_a \int \vec{v} f_a d^3 v \quad (2.28)$$

Considering the fluid model as a whole, it becomes evident that, although the continu-

ity equation governs the evolution of the zeroth-order moment, its formulation requires knowledge of terms such as the first-order moment $\vec{u}_a$. Similarly, the momentum balance equation describes a first-order moment but introduces the higher-order quantity $\underline{P}_a$, the total pressure tensor. The same pattern holds for the energy balance equation, which, despite being an equation for a second-order moment, depends on the third-order quantity $\vec{q}_a$. The fluid equations therefore form a hierarchy in which each equation depends on moments of higher order, ultimately generating an infinite chain of coupled equations. As a consequence, the multi-fluid model is intrinsically non-closed and requires the introduction of an appropriate closure [40].

The choice of closure depends on the plasma regime under consideration. One of the most widely adopted in plasma physics is the *Braginskii closure* [42], which applies to a collisional, fully ionized plasma composed of electrons and a single ion species in the presence of electromagnetic fields. This closure is based on the *relaxation hypothesis*, according to which binary Coulomb collisions occur sufficiently frequently to drive the electron and ion distribution functions toward quasi-Maxwellian distributions.

These conditions are generally well satisfied in the boundary plasma, but not in the sheath, which is characterized by strong gradients and low collisionality. Therefore, the validity domain of the fluid model typically ends at the sheath entrance, where appropriate *sheath boundary conditions* can be applied.

2.3. Global (0D) plasma models

Global models represent the final level of simplification in the hierarchy of theoretical plasma models. They are based on the volume averaging of plasma properties, thereby neglecting spatial variations, anisotropies, and other spatially resolved phenomena. Consequently, they are often referred to as 0D or *point models*, as an entire three-dimensional system is reduced to a single representative point where all properties are described by scalar quantities [43].

Despite the limitations of a zero-dimensional description, in which transport effects are neglected, several advantages arise from the use of this type of model. In fact, at a very low computational cost, global models provide estimates of the main plasma parameters, such as species densities and temperatures. Their reduced complexity enables the inclusion of detailed plasma chemistry, allowing the identification of dominant reactions and the evaluation of plasma composition. Moreover, the underlying physical mechanisms and the relationships among key plasma parameters generally emerge more clearly than in higher-dimensional models, making it possible to study their evolution across different

plasma regimes [43]. Global models therefore represent a fast and practical tool for estimating plasma parameters, composition, and dynamics, at the expense of spatial effects resolution.

The model can be derived directly from the multi-fluid equations. The assumption of plasma homogeneity allows all spatial derivatives to be neglected. As a result, the governing equations reduce to time-dependent balance equations, constituting a system of coupled, nonlinear differential equations. This system is composed, at minimum, of one particle balance equation for each species involved, the charge balance equation, and the power balance equation for the electron population. When the ion temperature T_i is not negligible with respect to the electron temperature, i.e. $T_i \sim T_e$, the ion power balance equation should also be included [43].

The global model equations are reported and analyzed in detail in Subsections 2.3.1 and 2.3.2. The modeling approaches available for the evaluation of the involved quantities are discussed in Subsection 2.3.3. Finally, the modeling of molecular plasmas is addressed in Subsection 2.3.4, with particular focus on hydrogen plasmas in Subsection 2.3.5.

2.3.1. Particle and charge balance

The particle balance equation for the a -th species can be derived from the fluid continuity equation (2.13). The source terms arising from reactions among particles and boundary exchange processes, which were neglected in the previous discussion, must now be reintroduced. By removing the spatial dependence, the 0D continuity equation is obtained [43]:

$$\frac{dn_a}{dt} = \sum_R S_{a,R} + \frac{A}{V} \Gamma_{boundary}^a + \frac{A}{V} \Gamma_{external}^a \quad (2.29)$$

where the subscript R labels the possible reactions in which each species can participate, V is the considered plasma volume, and A its surface area. The term $S_{a,R}$ ($\text{m}^{-3}\text{s}^{-1}$) represents the net volumetric particle source rate, accounting for both particle production and loss, associated with reaction R . The term $\Gamma_{boundary}^a$ ($\text{m}^{-2}\text{s}^{-1}$) represents the net particle flux entering the considered plasma volume through its boundaries. These boundaries may consist of virtual surfaces within the plasma, physical walls, or both. In the particular case where the volume of interest extends up to a wall, a wall flux term Γ_{wall}^a is included in the boundary contribution. Finally $\Gamma_{external}^a$ ($\text{m}^{-2}\text{s}^{-1}$) accounts for the possible presence of external particle sources or sinks, such as gas injection or pumping.

The particle balance equation is usually solved only for ionic (n_i) and neutral (n_g) species, while the electron density is evaluated through the charge balance equation by assuming

quasi-neutrality:

$$n_e = \sum_i \frac{n_i q_i}{e} \quad (2.30)$$

The source terms $S_{a,R}$ include all collisional reactions involving other plasma species, comprising both elastic and inelastic scattering processes. The latter may result either in excitation of the internal degrees of freedom of the interacting particles or in actual chemical or physical reactions, destroying the reactant particles and generating the corresponding products. Each source term can be expressed as³ [45]:

$$S_{a,R} = (\nu_{a,R}^p - \nu_{a,R}^d) K_R \prod_{a=\text{reactants}} n_a^{\nu_{a,R}^d} \quad (2.31)$$

where $\nu_{a,R}^p$ and $\nu_{a,R}^d$ are the stoichiometric coefficients of the products and reactants, respectively, and K_R (in m^3s^{-1}) is the energy-dependent *rate coefficient* or reactivity.

The definition of the rate coefficients can be recalled from the introductory Section 1.1. They describe the probability of a reaction R occurring among reactants of particle densities n_a , such that, for a binary collision, the reaction rate is given by $R = K_R n_a n_b$. They are computed from cross-section data by averaging the quantity $\langle \sigma(v)v \rangle$ over an appropriate velocity distribution function.

For a binary reaction between two generic particles, the reactivity can be derived by assuming Maxwellian velocity distributions, as done by Wauters *et al.* [46]:

$$K_R(T_1, T_2) = \int_0^\infty \sigma_R(u) u \hat{f}(T_1, T_2, u) d\epsilon = \sqrt{\frac{2}{\pi}} \left(\frac{m^*}{eT^*} \right)^{3/2} \int_0^\infty u^3 \sigma_R(u) \exp \left[-\frac{m^* u^2}{2eT^*} \right] du \quad (2.32)$$

where T_1 and T_2 are the Maxwellian temperatures of the interacting particles expressed in eV, m_1 and m_2 their masses in kg, $T^* = \frac{T_1 m_2 + T_2 m_1}{m_1 + m_2}$ is the reduced temperature and $m^* = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass. The quantity $u = |\vec{v}_1 - \vec{v}_2|$ denotes the relative impact velocity in m/s, while $\sigma(u)$ is the velocity-dependent reaction cross section in m^2 .

In the particular case of electron-impact reactions with atoms or molecules, the reduced mass and reduced temperature can be approximated by the corresponding electron quantities because of the large mass difference. Analogously, the relative velocity u reduces to the electron velocity v , owing to the much larger inertia of the heavy particles. Therefore,

³The same expression can also be reformulated in matrix form, which is particularly well suited for the numerical implementation of the model, as proposed by Body *et al.* [44].

the expression for the reaction rate coefficient becomes [41]:

$$K_R(T_e) = \left(\frac{m_e}{2\pi e T_e} \right)^{3/2} \int_0^\infty \sigma_R(v) v \exp \left[-\frac{m_e v^2}{2e T_e} \right] 4\pi v^2 dv \quad (2.33)$$

The same expression can equivalently be written in terms of the electron energy distribution function (EEDF), recalling that for $v = \sqrt{2e\epsilon/m_e}$ the cross section can also be expressed as a function of the electron energy $\sigma(\epsilon)$ [44]:

$$K_R(T_e) = \int_0^\infty \sigma_R(\epsilon) v(\epsilon) \hat{f}(T_e, \epsilon) d\epsilon = \int_0^\infty \sigma_R(\epsilon) \sqrt{\frac{8e\epsilon^2}{\pi m_e T_e^3}} \exp \left[-\frac{\epsilon}{T_e} \right] d\epsilon \quad (2.34)$$

It is important to note that the assumption of a Maxwellian distribution may limit the applicability of the resulting equations. Under certain conditions – particularly for the electron population – the distribution function may significantly deviate from a Maxwellian. This can occur, for example, at very low pressures, in predominantly capacitively coupled discharges, or in the presence of strong DC magnetic fields. In such cases, it may be necessary to explicitly account for the non-Maxwellian nature of the electron energy distribution function in the model formulation [47]. Similarly, ionic species are not necessarily in thermal equilibrium and may therefore deviate from a Maxwellian energy distribution function; despite this, they are often modeled as Maxwellian populations [43].

The evaluation of rate coefficients is intrinsically affected by several sources of uncertainty. For each reaction, the corresponding cross section must be selected from multiple databases and literature sources, where it is often difficult to trace the original experimental or theoretical data and assess their reliability. Moreover, despite the large amount of data available in existing databases, some reactions may still lack complete information, making it necessary to estimate reactivities or cross sections. Furthermore, any analytical expression for a reaction rate coefficient necessarily represents an approximation of the complex interactions occurring at the microscopic level, which require quantum-mechanical calculations for an accurate description [43].

2.3.2. Power balance

The power balance equation is obtained from the corresponding fluid equation (2.15) in the same way as the particle balance equation, reintroducing the source terms arising from particle reactions and boundary exchange processes. In the most general case, it can

be written for each species included in the model (adapted from [44]):

$$\frac{d}{dt} \left(\frac{3}{2} e n_a T_a \right) = P_{input}^a + P_{coll}^a + P_{boundary}^a \quad (2.35)$$

where the species temperature T_a is expressed in eV. P_{input}^a (Wm^{-3}) is the input power density, which is non-zero only if the considered species is involved in the specific heating mechanism employed in the system, and may eventually be a function of time. P_{coll}^a (Wm^{-3}) represent the net energy gain or loss due to inelastic and elastic collisions between the a -species and the other particles. Finally, $P_{boundary}^a$ (Wm^{-3}) accounts for the energy loss or gain resulting from particle exchange at the boundaries.

In many applications, electron-heated plasmas are considered with $T_e \gg T_n \simeq T_i$. Therefore, only the electron power balance is considered, while the neutral and ion temperatures are assumed to be constant or empirically determined. The electron energy balance is then written as

$$\frac{d}{dt} \left(\frac{3}{2} e n_e T_e \right) = P_{input}^e + P_{coll}^e + P_{boundary}^e \quad (2.36)$$

In the most general case the collision term P_{coll}^e (Wm^{-3}) can be expressed as [43]:

$$P_{coll}^e = \sum_R E_R K_R n_R n_e \quad (2.37)$$

where R includes elastic collisions, ionization, excitation and chemical reactions, while E_R (J) represents the energy loss or gain associated with the corresponding process. In the particular case of elastic collisions, the exchanged energy $E_{R,el}$ can be estimated analytically as

$$E_{R,el} = 3 \frac{m_e}{m_a} e (T_e - T_a) \quad (2.38)$$

$$T_e \gg T_a \Rightarrow E_{R,el} \simeq 3 \frac{m_e}{m_a} e T_e \quad (2.39)$$

2.3.3. Charged particles and power losses at the wall

Among the possible boundary losses, wall losses constitute a particularly relevant category. In the following, two cases are considered, corresponding to magnetically confined and unconfined plasmas.

When the plasma is not magnetically confined, it comes into direct contact with the solid walls, leading to the formation of an electrostatic sheath. The electron and ion fluxes

through the sheath can be evaluated according to the Bohm criterion. For the i -th ionic species, the flux corresponds to Equation 1.35; therefore, by ambipolarity, the electron flux is given by

$$\Gamma_{wall}^e = \sum_i \Gamma_{wall}^i = \sum_i n_{se,i} u_{B,i} \quad (2.40)$$

where $u_{B,i}$, expressed in m/s, is the Bohm velocity of the i -th ion species, and $n_{se,i}$ is its density at the sheath edge. Once the electron flux is known, the electron power losses at the wall, P_{wall}^e , can be evaluated using the electron heat flux density at the sheath entrance defined in Equation 1.39:

$$P_{wall}^e = \frac{A}{V} e \Gamma_{wall}^e (2T_e + |V_{sf}| + |V_{pre-sheath}|) \quad (2.41)$$

Strictly speaking, the electron heat flux density at the sheath edge and the one effectively reaching the wall are not the same quantity. As discussed in Subsection 1.3.2, only a fraction of the power entering the sheath is ultimately deposited onto the wall, while the remaining part is transferred to the ions through sheath acceleration processes. Nevertheless, from the point of view of the electron energy balance, the net loss for the electron population is still given by the heat flux density at the sheath entrance. For this reason, throughout this work, such a contribution is conventionally referred to as a *wall loss*, although this terminology is not strictly rigorous from an energetic standpoint.

The evaluation of Γ_{wall}^e requires knowledge of the ion densities at the sheath edge. Unfortunately, by definition, a global model is not able to capture any spatial dependence of the plasma parameters; therefore, these densities are not computed internally and must be modeled appropriately. Different approaches can be found in the literature. In many cases, the difference between the sheath-edge density $n_{se,i}$ and the bulk density n_i is accounted for by introducing an *effective area* $A_{eff,i}$ for ion losses, such that the wall loss rate can be expressed as

$$R_{wall}^i = u_{B,i} n_i \frac{A_{eff,i}}{V} \quad (2.42)$$

Lieberman and Lichtenberg in *Principles of Plasma Discharges and Materials Processing* [41], report the following approach based on the solution of the *ambipolar diffusion problem*.

For a cylindrical geometry, with R and L denoting the cylinder radius and length, respectively, and λ_i the ion-neutral mean free path, three different *pressure regimes* can be identified, each corresponding to a different evaluation of the effective area.

For $\lambda_i \gtrsim (R, L)$, the system is in the *low-pressure regime*, also known as the *Langmuir*

regime. In this case, ion transport is nearly collisionless and is well described by an *ion free-fall profile* within the bulk plasma. This profile is relatively flat near the plasma center and decreases close to the sheath edge, with $n_{se}/n_i \approx 0.5$ for $R \gg L$ and $n_{se}/n_i \approx 0.4$ for $L \gg R$. Here, n_{se}/n_i corresponds to A_{eff}/A .

When $(R, L) \gtrsim \lambda_i \gtrsim (T_i/T_e)(R, L)$, the system is in the *intermediate-pressure regime*, also known as the *variable-mobility regime*. In this situation, the effective area is expressed as $A_{eff} = 2\pi R^2 h_l + 2\pi R L h_R$, where h_l and h_R are the *edge-to-center density ratios* in the axial and radial directions, respectively, defined as [48]:

$$\begin{cases} h_l = \frac{n_{se,l}}{n_i} \approx 0.86 \left(3 + \frac{L}{2\lambda_i} \right)^{-1/2} \\ h_R = \frac{n_{se,R}}{n_i} \approx 0.80 \left(4 + \frac{R}{\lambda_i} \right)^{-1/2} \end{cases} \quad (2.43)$$

$$\quad (2.44)$$

Finally for $\lambda_i \lesssim (T_i/T_e)(R, L)$, the *high-pressure regime*, or *constant diffusion coefficient regime*, is reached. In this case, the heuristic solution proposed by Lee and Lieberman [49], which smoothly connects all three regimes, can be considered. Defining D_a as the ambipolar diffusion coefficient, J_1 as the first-order Bessel function, and χ_{01} as the first zero of the zero-order Bessel function, h_l and h_R are given by

$$\begin{cases} h_l = \frac{n_{se,l}}{n_i} \approx 0.86 \left(3 + \frac{L}{2\lambda_i} + \left(\frac{0.86 L u_B}{\pi D_a} \right)^2 \right)^{-1/2} \\ h_r = \frac{n_{se,r}}{n_i} \approx 0.80 \left(4 + \frac{R}{\lambda_i} + \left(\frac{0.80 R u_B}{\chi_{01} J_1(\chi_{01}) D_a} \right)^2 \right)^{-1/2} \end{cases} \quad (2.45)$$

$$\quad (2.46)$$

This approach is also valid for planar geometries, where the formulation for h_l is applied to all three dimensions of a parallelepiped.

In the case of a magnetically confined plasma, particles are lost to the wall only if they succeed in escaping magnetic confinement. Different approaches can be adopted to describe the losses in the confinement direction depending on the specific configuration [41]. Among them, the diffusion approximation for radial transport discussed in Subsection 1.3.1 can be exploited to evaluate the flux of particles across magnetic field lines, ultimately escaping confinement and reaching the wall. Denoting by x the direction orthogonal to the

magnetic field lines (i.e., the radial direction), the diffusion equation can be written as

$$v_{\perp,i} n_i = -D_{\perp} \frac{\partial n_i}{\partial x} \quad (2.47)$$

where $D_{\perp}$ is the anomalous diffusion coefficient. Defining the density decay length as $\lambda_n = -\left(\frac{1}{n_i} \frac{\partial n_i}{\partial x}\right)^{-1}$, the cross field velocity can be obtained as $v_{\perp} = D_{\perp}/\lambda_n$ [22]. This quantity can be regarded as the effective radial velocity at the boundary, yielding an escaping particle flux given by

$$\Gamma_{wall,\perp}^i = v_{\perp} n_i = \frac{D_{\perp}}{\lambda_n} n_i \quad (2.48)$$

This approach may be particularly useful for comparisons with other theoretical and numerical models, including higher-dimensional ones, that use the anomalous transport coefficient as an input parameter. As an example, Tonello *et al.* [50], employed this method in a modeling study of helium plasmas in the GyM linear plasma device, where the developed global model was compared with the 2D SOLPS-ITER code.

For confined plasmas, the power losses can be evaluated as:

$$P_{wall,\perp}^e = \frac{3}{2} e T_e \Gamma_{wall,\perp} \quad (2.49)$$

Similarly, suitably evaluated particle and energy confinement times can also be employed [46, 51–54]:

$$\Gamma_{wall,\perp}^a = \frac{n_a}{\tau_{p,a}} \quad P_{wall,\perp}^a = \frac{3}{2} \frac{n_a T_a}{\tau_{E,a}} \quad (2.50)$$

Along the unconfined direction, diffusion proceeds in the same way as in the absence of an applied magnetic field; therefore, the same treatment applies [41].

2.3.4. Distinctive features of molecular plasma modeling: neutral-wall recombination, vibrational states and electronegative effects.

Within the general framework of the global model described above, some peculiarities arise in the specific case of molecular plasmas. Their chemistry and the variety of involved species are considerably richer, making the overall dynamics more complex. The particular phenomena that occur exclusively, or predominantly, in this kind of plasma are described in this section.

Neutral-wall recombination

Molecules in plasmas typically undergo dissociation processes, ultimately leading to the formation of atomic species, which can be either neutrals or ions. Neutral atoms diffuse freely inside the plasma and can reach the walls, where they may be absorbed and recombine into molecular neutrals. For non-reentrant discharge geometries (e.g., cylinders and rectangular boxes), the rate coefficient for neutral losses at the wall can be evaluated using the simple formulation introduced by Chantry [55]. For particles A diffusing through collisions with particles B , characterized by diffusion coefficient D_{AB} , temperature $T_A = T_B = T$, reduced mass m^* , and mean relative speed $\bar{v}_{AB} = \sqrt{8eT/\pi m^*}$, the wall-loss rate coefficient is expressed as [41]:

$$K_{A,loss} = \left[\frac{\Lambda_0^2}{D_{AB}} + \frac{2V(2 - \gamma)}{A\bar{v}_{AB} \gamma} \right]^{-1} \quad (2.51)$$

Here, Λ_0 is the diffusion length, V the discharge volume, A the surface area for losses, and γ the wall-loss probability. The diffusion coefficient is computed as [41]:

$$D_{AB} = \frac{\pi}{8} \lambda_{AB} \bar{v}_{AB} \quad (2.52)$$

where $\lambda_{AB} = 1/n_B \sigma_{AB}$ is the mean free path, with the collision cross section estimated using the *hard-sphere* approximation, $\sigma_{AB} \approx \pi(r_A + r_B)^2$.

From this relation, for a given neutral atomic species X , the commonly adopted formulation for the neutral wall-recombination rate coefficient [44, 47, 56–59] can be obtained by introducing the wall recombination probability γ_r :

$$K_{X,loss} = \left[\frac{\Lambda_0^2}{D_X} + \frac{2V(2 - \gamma_r)}{A\bar{v}_X \gamma_r} \right]^{-1} \quad (2.53)$$

The value of γ_r depends on the wall material and can be evaluated through experimental measurements.

Vibrational states and collisional energy loss

Another major difference between molecular and atomic plasmas lies in the available excited states. In all plasmas, inelastic collisions may lead to the excitation of internal degrees of freedom. However, in atomic plasmas only electronic excitation levels are available, whereas molecular plasmas also exhibit vibrational and rotational excitations. An accurate description of these excitation processes may be fundamental, since they can

significantly affect the power balance equation by constituting a non-negligible power-loss channel. Furthermore, excited molecules can open preferential pathways for specific reactions. For example, dissociative electron attachment in hydrogen is strongly enhanced when the molecule is vibrationally excited.

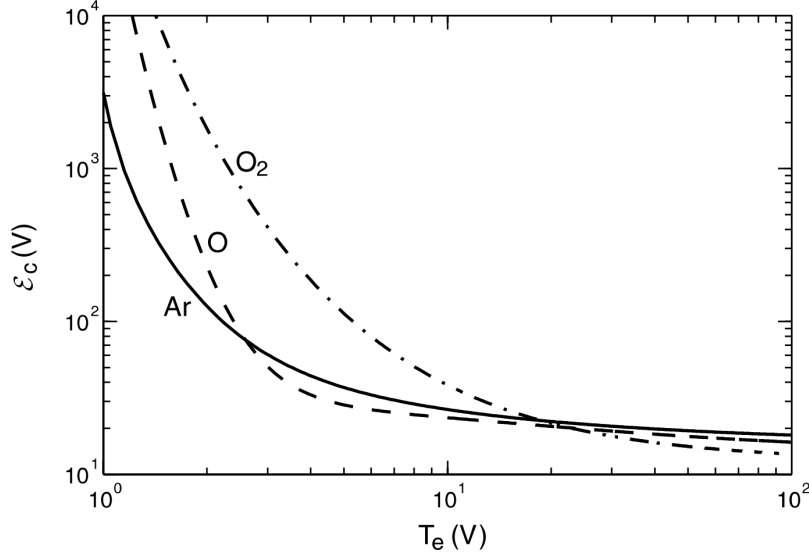


Figure 2.3: Collisional energy loss per electron-ion pair created, ϵ_c , as a function of the electron temperature T_e in argon and oxygen plasmas. Adapted from [41]; data compiled by Gudmundsson [60].

When molecules are involved, the evaluation of the electron collisional power-loss term P_{coll}^e becomes particularly challenging due to the large number of possible excitation processes following a collision event. Lieberman and Lichtenberg [41] report a modeling approach widely adopted in the literature for molecular plasmas [47, 56–60]. This method introduces the *collisional energy loss* per electron-ion pair created, $\epsilon_c(T_e)$:

$$\epsilon_c^{(X)} = \epsilon_{iz}^{(X)} + \sum_i \epsilon_{ex,i}^{(X)} \frac{k_{ex,i}^{(X)}}{k_{iz}^{(X)}} + \frac{k_{el}^{(X)}}{k_{iz}^{(X)}} \frac{3m_e}{m^{(X)}} T_e \quad (2.54)$$

where $\epsilon_{iz}^{(X)}$ is the ionization energy of species X , $\epsilon_{ex,i}^{(X)}$ and $k_{ex,i}^{(X)}$ are the excitation energy and rate coefficient for the i -th excitation process of species X , respectively, $k_{el}^{(X)}$ is the elastic scattering rate coefficient of species X , m_e is the electron mass and $m^{(X)}$ is the mass of species X . Accordingly, the last two terms in the equation represent the vibrational and elastic energy loss rates, respectively, normalized to the ionization rate. The collisional

power losses can therefore be written as:

$$P_{coll}^e = en_e \sum_X n^{(X)} \epsilon_c^{(X)} k_{iz}^{(X)} \quad (2.55)$$

Figure 2.3 reports the collisional energy-loss curves for an atomic gas (argon) and a molecular gas (oxygen), showing that ϵ_c is generally a factor of 2-10 larger in molecular gases than in atomic gases for electron temperatures below approximately 7 eV.

During interactions with the walls, vibrationally excited molecules typically de-excite toward lower-energy states. The corresponding rate coefficient can be evaluated using the same formulation adopted for neutral wall recombination in Equation 2.53, replacing the recombination probability γ_r with an appropriate quenching probability γ_Q .

Electronegativity effects

Finally, another important peculiarity of molecular plasmas is the possible formation of negative ions. In this case, the plasma is referred to as *electronegative*. Negative ions behave considerably differently from positive ions. Owing to the positive plasma potential, they are confined within the plasma bulk and are not efficiently lost to the walls as positive ions are. As a consequence, the plasma stratifies into an electronegative core surrounded by an electropositive halo [47]. The Bohm criterion must therefore be modified to account for the reduced ion Bohm velocity caused by the presence of negative ions. For low-pressure plasmas, Braithwaite and Allen [61] derived the modified Bohm criterion:

$$u_B = \sqrt{\frac{eT_e(1 + \alpha_s)}{M(\alpha\gamma_- + 1)}} \quad (2.56)$$

where M_- is the negative ion mass, $\alpha = n_-/n_e$ is the mean electronegativity, α_s is the electronegativity at the sheath edge, and $\gamma_- = T_e/T_-$. The generalized Bohm criterion also leads to a modified plasma potential expression [56]:

$$V_p = \frac{1}{2} \frac{1 + \alpha_s}{1 + \alpha_s \gamma_-} T_e \quad (2.57)$$

Several attempts have been made to describe the impact of electronegativity within the framework of global models. One of the most successful approaches for describing sheath-edge densities in electronegative plasmas was proposed by Kim *et al.* in 2006 [62]. They identified three distinct electronegativity regimes: (a) a two-region plasma composed of a low-pressure electronegative core with a parabolic density profile and a low-pressure

electropositive edge; (b) a single-region parabolic electronegative plasma occurring at low pressures and high electronegativity; and (c) a one-region flat-topped electronegative plasma occurring at high pressures and high electronegativity. For weakly electronegative plasmas, such as those considered in this thesis, regime (b) can be neglected. Therefore, for a high-aspect-ratio plasma, $2R \gg L$, the edge-to-center density ratios for the intermediate-pressure regime discussed in Subsection 2.3.3 can be corrected to account for electronegativity effects. For the regimes (a) and (c) the following expressions are considered:

$$h_{l,a} = 0.86 \left[\sqrt{3 + \eta l_p / \lambda_+} \right]^{-1} \frac{1}{1 + \alpha_0} \quad h_{l,c} \simeq \left[\gamma_-^{1/2} + \left(\frac{\gamma_+ n_*}{n_{-0}} \right)^{1/2} \right]^{-1} \quad (2.58)$$

where $l_p = L/2$ is the plasma chamber half-width, $\gamma_+ = T_e/T_+$ is the electron-to-positive-ion temperature ratio, and

$$n_* = \frac{15}{56} \frac{\eta^2}{k_{rec} \lambda_i} v_i \quad (2.59)$$

with v_i being the mean thermal velocity of positive ions and $k_{rec} \simeq 5 \times 10^{-14} \text{ m}^3\text{s}^{-1}$ the mutual-neutralization rate coefficient in the plasma bulk.

To extend Kim's results to a finite cylindrical geometry, for which radial losses of charged species may be non-negligible, the radial ion flux factor h_R must also be evaluated. Since $h_{l,c}$ is independent of the chamber dimensions, it is assumed to be identical in the radial direction, namely $h_{l,c} = h_{R,c} = h_c$. By contrast, $h_{R,a}$ can be expressed as:

$$h_{R,a} = 0.8 \left[\sqrt{4 + \eta R / \lambda_+} \right]^{-1} \frac{1}{1 + \alpha_0}. \quad (2.60)$$

The contributions from the different regimes are finally combined into a single expression valid over the entire range of considered conditions, following the ansatz proposed by Monahan and Turner [63]:

$$h_{(l,R)}^2 = h_{(l,R),a}^2 + h_c^2. \quad (2.61)$$

These ion-flux factors are subsequently used to define the effective area for ion losses. The effective area A_{eff} obtained in this way already accounts for the modification of the Bohm velocity induced by the presence of negative ions near the sheath edge. Therefore, the standard Bohm velocity formulation should still be used when calculating wall losses.

2.3.5. State of the art in Hydrogen 0D models: open points in isotopic adaptation

In the context of nuclear fusion, hydrogenic plasmas are of particular relevance since, as discussed in Section 1.1, the preferred reaction is the D-T reaction, involving the two hydrogen isotopes deuterium and tritium.

Different approaches to the global modeling of hydrogen plasmas can be found in the literature. One of the earliest examples of a volume-averaged approach for hydrogen discharges was presented by Fukumasa *et al.* in 1985 [64], who developed a particle and charge balance model including H, H₂, H₂⁺, and H₃⁺, together with seven chemical reactions. Later, Zorat *et al.* (2000) [65] extended this framework by including a power balance equation.

Early models typically neglected the formation of negative ions or treated them with limited accuracy, assuming their concentration to be small. This is also the case for the works of Yazawa *et al.* (2006) [66] and Kimura and Kasugai (2010) [67]. Over time, however, the accurate modeling of the H⁻ density became increasingly important, since negative hydrogen ion sources emerged as a key technology for plasma heating in thermonuclear reactors, producing intense energetic neutral beams to be injected into the plasma core [68]. Among the first studies addressing this aspect are the works of Mosbach (2005) [69] and Pagano *et al.* (2007) [70].

In this context, the work of Hjartarson *et al.* (2010) [56] is particularly relevant, as it paved the way for several subsequent studies. They developed a global model for a low-pressure (1-100 mTorr), high-density hydrogen discharge diluted with argon, applying it to investigate the effects of argon on the dissociation fraction, electron density, relative ion densities, electron temperature, and dominant reaction mechanisms. The model included the fourteen lowest vibrational levels of molecular hydrogen, discussing their relative contributions and highlighting the importance of vibrationally excited states as pathways for dissociative attachment.

In 2016, the work of Hjartarson *et al.* [56] was used as a reference for the development of a pure hydrogen model by Samuelli and Corr [47]. Their global model was developed to predict the behavior of electrons, ground-state atomic and molecular hydrogen, the three positive ion species (H⁺, H₂⁺, and H₃⁺), a single negative ion species (H⁻), and fourteen vibrationally excited states of molecular hydrogen (H₂($\nu = 1-14$)). Compared with previous works, updated kinetic data sources were employed to calculate reaction rates, an extension to low-aspect-ratio reactor geometries was introduced, and the Rydberg states of H₂

were included as an excitation channel for vibrational states. The model was validated against experimental results obtained in a planar inductively coupled *gaseous electronics conference (GEC) reference cell* [71] and was subsequently applied to the *MAGPIE linear helicon reactor* [72].

Among the most recent works, it is worth mentioning the model developed by Yang *et al.* (2016) [58, 59] for pure hydrogen plasmas, benchmarked against the *Global Enhanced Vibrational Kinetic Model (GEVKM)* [73] and validated using the *radio-frequency* source developed by Gao *et al.* [74]; the work of Body *et al.* (2018) [44] on nitrogen-hydrogen mixtures, aimed at investigating the effects of nitrogen impurity seeding in tokamak power exhaust scenarios; the model by Wu *et al.* (2020) [51] for the investigation of ion sources producing intense H^+ , H_2^+ , and H_3^+ beams; and the recent work by Aghbolaghi *et al.* (2024) [52].

By contrast, a general lack of dedicated modeling studies is observed in the literature for hydrogen isotopes. In many cases, global hydrogen plasma models are applied to experimental devices operating with deuterium, while only hydrogen chemistry and physics is explicitly considered in the simulations. Such an approximation may provide a rough estimate if at least the mass difference is accounted for. Nevertheless, the resulting plasma composition may not be accurate, since additional isotope effects can play a significant role, particularly through differences in cross-section data and vibrational spectra. The latter depend not only on the molecular species itself but also on the masses of the nuclei involved and therefore on the specific isotope. In particular, the electronic ground state of deuterium possesses twenty-one vibrationally excited levels, compared with fourteen for hydrogen. Consequently, the inclusion of vibrational states in the model requires the replacement of all cross sections involving such states. An accurate treatment of vibrational kinetics is believed to be especially important for reliable predictions of negative ion densities [75, 76].

The existence of an isotope effect in negative hydrogen ion formation through dissociative electron attachment was theoretically predicted by Demkov [77] and by Chen and Peacher [78], and later demonstrated experimentally by Schulz and Asundi [79] and by Rapp *et al.* [80]. Allan and Wong [81], and later Orient and Chutjian [82], experimentally showed that the dissociative electron attachment cross sections depend on the rovibrational state of the molecule and are isotope dependent. Consequently, negative ion densities are expected to differ significantly in deuterium plasmas. In particular, the reduced volume production rate of negative deuterium ions in deuterium plasmas, compared with the production rate of negative hydrogen ions in hydrogen plasmas, is generally attributed to two main factors: (a) the dissociative electron attachment cross sections for the differ-

ent rovibrationally excited states of D_2 are lower than the corresponding cross sections for H_2 ; (b) deuterium plasmas exhibit a higher plasma potential, associated with higher electron temperatures and heavier positive ions [75].

It must be mentioned that, due to the widespread use and recognized value of global models within the plasma research community, a number of well-established codes are available for solving global models under user-defined conditions and for different plasma chemistries [43]. Nevertheless, most of these codes are not open source and typically require the user to provide the reaction sets and corresponding cross sections, thus not fully overcoming the issue of isotope dependence in hydrogen plasma models. Among the most established tools are the *GlobalKin* code [83], which solves global models using prescribed reaction rate coefficients and also includes a module for calculating the electron energy distribution function (EEDF); the *ZDPlasKin* code [84], capable of computing the time evolution of species densities for user-defined reaction schemes, including EEDF calculations and gas temperature evaluation; and the *PLASIMO* toolkit [45, 85], which provides a wide range of modules, including electromagnetic solvers, flow solvers, transport coefficient calculations, radiation transport, and generation of orthogonal curvilinear coordinate systems.

2.4. Numerical modeling: the example of SOLPS-ITER code

Theoretical plasma models ultimately lead to sets of balance equations for the plasma parameters, forming systems of coupled non-linear differential equations. Except for highly simplified configurations, these systems can rarely be solved analytically, and numerical approaches are therefore generally employed. Depending on the specific application, several established simulation codes are available and widely used within the plasma physics community.

In the context of nuclear fusion, one of the most established and widely adopted tools is the *SOLPS-ITER* code package (*Scrape-Off Layer Plasma Simulation*), which is specifically designed for simulations of the plasma edge region in magnetic confinement devices. The most recent version of the code is maintained by the *ITER Organisation (IO)* [37].

The structure and operating principles of SOLPS-ITER are described in Section 2.4.1, while Section 2.4.2 discusses in detail the modeling approach adopted for molecular ions and the related open issues.

2.4.1. Code structure

SOLPS-ITER is built upon the self-consistent coupling of two distinct modules: B2.5, a two-dimensional multi-fluid plasma solver, and EIRENE, a fully three-dimensional Monte Carlo code dedicated to neutral transport. Each module can be run independently in standalone mode, or jointly in a coupled B2.5-EIRENE simulation. Although the code was originally developed for tokamak geometries, its applicability has since been extended to linear devices as well [86].

The B2.5 module traces its origins to the B2 code developed by Braams [87] and Baelmans [88]. It solves a set of modified Braginskii fluid equations governing the plasma: a continuity equation and a parallel momentum equation for each ion species, separate energy balance equations for electrons and each ion species - the latter assuming equal temperatures across all ion species - and a current continuity equation, derived under the quasi-neutrality assumption. Being a non-turbulent mean-field code, B2.5 evolves the plasma on time scales well exceeding those characteristic of turbulent fluctuations, whose net transport effects are instead captured through anomalous cross-field diffusion and convection coefficients [89]. The spatial domain is a two-dimensional poloidal plane, with toroidal symmetry assumed throughout, this is known as a 2.5D approach.

While a fluid treatment of neutral species may be adequate under specific conditions, capturing the full complexity of atomic and molecular processes on a plasma background generally demands a kinetic description. EIRENE, originally developed by Reiter [90], fulfills this role as the kinetic neutral transport module of SOLPS-ITER. It operates as a fully 3D Monte Carlo code, in which a population of test particles is launched from prescribed sources with given velocity and angular distributions, and then tracked along their trajectories until they are lost through reactive events. The probability of each interaction is determined by its cross-section, sourced from external atomic and molecular databases [89].

The two modules are coupled at every time step through an iterative exchange of information. B2.5 first advances the fluid equations using an implicit Euler scheme, yielding a background plasma solution that is subsequently passed to EIRENE. The latter then simulates neutral particle trajectories within this background, computing the resulting plasma-neutral interactions. The corresponding source and sink terms for particles, momentum, and energy are fed back into B2.5, which recomputes the plasma solution, thus closing the coupling loop for the next iteration [86].

Figure 2.4 schematically illustrates the workflow of the SOLPS-ITER code package. In particular, the coupling between the B2.5 and EIRENE modules is shown on the right-

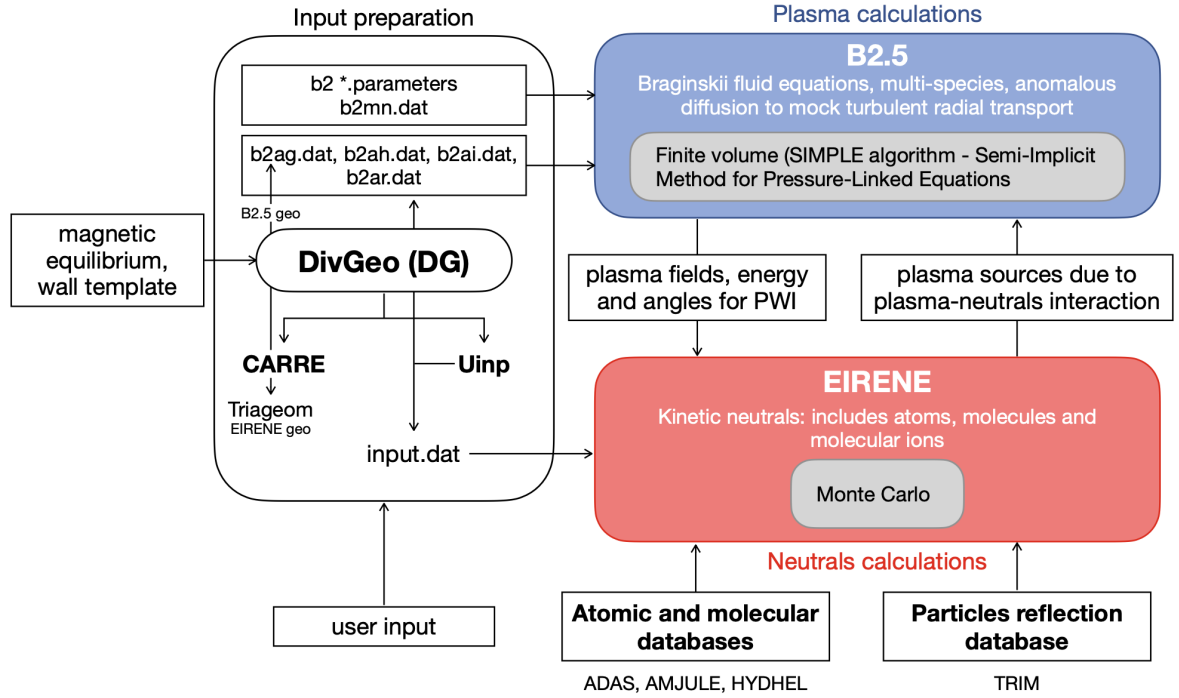


Figure 2.4: Simplified SOLPS-ITER workflow, from [91].

hand side, while the left-hand side includes auxiliary tools (e.g., DivGeo, Carre, and Uinp) devoted to geometry definition, mesh generation, pre-processing, and post-processing tasks.

The main steps required to set up a SOLPS-ITER simulation can be summarized as follows [38]:

- Definition of the simulation geometry using the **DivGeo** utility, including the specification of vacuum vessel walls, material properties, pumping locations, and plasma species;
- Generation of the plasma mesh through the **Carre** mesh generator, which produces a structured quadrangular grid for the plasma solver. The mesh extends from the edge of the confined plasma region to the first tangency line with a limiting wall structure;
- Creation of the input files using the **Uinp** utility, which processes the previously defined data and generates the corresponding EIRENE input files, together with part of the B2.5 input;

- Generation of the neutral particle mesh by means of the **Tria** and **Triageom** programs. These tools construct an unstructured triangular grid covering both the region meshed by Carre and the outer SOL domain up to the vacuum vessel wall;
- Definition of the physical input parameters. Plasma quantities are provided through dedicated input files and translated into the internal format required by B2.5.

The main input files commonly employed in a SOLPS-ITER simulation, through which the user specifies the relevant physical and numerical parameters, are listed below:

- `b2ag.dat` defines the geometry of the problem, including the grid dimensions and mesh structure;
- `b2ah.dat` contains information about the fluid plasma species included in the simulation;
- `b2ai.dat` provides the initial plasma state;
- `b2ar.dat` specifies the density and temperature ranges used to generate the atomic physics tables from the selected databases;
- `input.dat` dictates the geometry, boundary materials, particle species, and atomic/molecular physics to be used in the EIRENE simulation;
- `b2mn.dat` is the main input file of the code, containing the general simulation setup, operational parameters, and switches enabling the use of additional customized input files;
- `b2.boundary.parameters` defines the boundary conditions adopted for the solution of the plasma fluid equations;
- `b2.neutrals.parameters` specifies settings related to the treatment of neutral particles;
- `b2.numerics.parameters` contains the numerical schemes and solver parameters used in the computation;
- `b2.transport.parameters` defines the anomalous transport coefficients for particle, momentum, and energy transport in the plasma;
- `b2.sources.profile` used to prescribe external particle, momentum, and energy source profiles.

2.4.2. Molecular ion modeling and open points in SOLPS-ITER simulations

Particularly relevant for the scope of this thesis work is the way molecular ions are handled in SOLPS-ITER.

Molecular species are not treated as individual populations by the multi-fluid module; instead, they are accounted for as *test ions* in the EIRENE module. Since ions are charged rather than neutral particles, their kinetic treatment would in principle require solving the full Boltzmann equation, including the contribution associated with the Lorentz force. For this reason, EIRENE does not explicitly follow the trajectories of test ions, but rather applies the *static approximation*, meaning that the next collision is assumed to occur at the particle birth location [89, 92]. This approximation is justified only when the considered test particle is *short-lived*, namely when its mean free path is much smaller than the characteristic spatial resolution, i.e. the computational grid cell dimensions [92]. Such a condition is generally satisfied for the plasma densities typically reached in the tokamak SOL; however, this is not necessarily the case in linear plasma devices, where the densities can be significantly lower [89]. Therefore, in the latter case, the validity of the static approximation should be carefully assessed.

In the specific case of hydrogen plasmas, the default simulation setup in SOLPS-ITER includes only H and H^+ as fluid species, whereas H_2^+ is treated exclusively as an EIRENE test ion, and neither H_3^+ nor H^- are included. The validity of the static approximation for H_2^+ should therefore be carefully verified before applying the model to linear plasma devices. For example, the approximation was shown to be valid for *Pilot-PSI*, a linear plasma device formerly operated at the *Dutch Institute for Fundamental Energy Research (DIFFER)* [92]. However, this machine is characterized by plasma densities of approximately 10^{20} - 10^{21} m^{-3} , which are higher than those typically achieved in many other linear plasma devices. Therefore, this result do not necessarily guarantee the validity of the approximation in lower-density operating conditions. In the case of GyM, for example, where plasma densities are as low as $n_e \leq 10^{17} \text{ m}^{-3}$, the validity of this approximation has already been questioned in an ongoing unpublished work by A. Villa [93], highlighting the need for a further verification.

The default set of reactions implemented in EIRENE is reported in Table 2.1. It is worth noting that vibrationally excited states of hydrogen molecules are not included as individual species, and consequently the related reactions are absent as well.

Table 2.1: List of atomic and molecular physics processes, with the corresponding databases, used in EIRENE.

ID	Reaction	Database
1	$H_2 + H^+ \rightarrow H_2 + H^+$	AMJUEL 0.3T [94]
2	$e^- + H \rightarrow 2e^- + H^+$	AMJUEL 2.1.5 [94]
3	$e^- + H_2 \rightarrow 2e^- + H_2^+$	AMJUEL 2.2.9 [94]
4	$e^- + H_2^+ \rightarrow 2e^- + 2H^+$	AMJUEL 2.2.11 [94]
5	$e^- + H_2 \rightarrow e^- + 2H$	AMJUEL 2.2.5g [94]
6	$e^- + H_2 \rightarrow e^- + H + H^+$	AMJUEL 2.2.10 [94]
7	$e^- + H_2^+ \rightarrow e^- + H + H^+$	AMJUEL 2.2.12 [94]
8	$e^- + H_2^+ \rightarrow 2H$	AMJUEL 2.2.14 [94]
9	$H + H^+ \rightarrow H^+ + H$	HYDHEL 3.1.8 [95]
10	$H_2 + H^+ \rightarrow H_2^+ + H$	AMJUEL 3.2.3 [94]
11	$e^- + H^+ \rightarrow H + \gamma$	AMJUEL 2.1.8 [94]

2.5. Thesis motivations and objectives

The discussion presented in Chapter 1 has highlighted the main challenges associated with the development of fusion technology. Still far from full maturity, it remains a highly active field of scientific investigation, in which experimental campaigns are increasingly complemented by modeling approaches. These have become indispensable for investigating physical phenomena and system properties that would otherwise be difficult, or impractical to study experimentally.

The central role of hydrogen in fusion research has been a recurring theme throughout this work. As discussed in Section 1.1, the D-T reaction is currently regarded as the most promising candidate for future fusion energy production and will be employed in ITER and, potentially, in future reactors. Hydrogenic plasmas are, however, characterized by considerable complexity owing to the wide range of physical and chemical processes involved. This complexity arises primarily from the molecular nature of hydrogen and from the isotopic effects associated with deuterium and tritium. As a result, the applicability and reliability of currently available modeling approaches and numerical tools for describing such plasmas must be carefully assessed.

Global models represent a valuable tool for addressing this complexity, as they allow a wide range of chemical reactions and physical processes to be included while enabling their mutual interplay to be investigated at a relatively modest computational cost. Additionally, their ability to estimate plasma and operational parameters can support experimental campaigns in two ways: predictively, by helping to set up the experiment, and

interpretively, by assisting in the analysis of the results.

As a modeling approach, global models are particularly well suited to the analysis of Linear Plasma Devices (LPDs). As discussed in Section 1.3, LPDs are valuable tools for investigating plasma-material interactions (PMI), including material erosion, fuel recycling, impurity production, redeposition, and the fundamental mechanisms underlying plasma detachment. They are therefore highly relevant to fusion research, where PMI constitute one of the major challenges to the realization of fusion energy. A comprehensive characterization of plasma parameters, in particular of plasma composition, is essential to support these studies, making the availability of a reliable modeling tool for estimating such quantities a matter of particular importance.

Global models are also characterized by inherent simplicity and a direct connection to the underlying plasma physics. These features make them well suited for identifying missing physical mechanisms or inadequate assumptions in higher-fidelity models and numerical codes. In this regard, Subsection 2.4.2 discussed an open issue concerning the modeling strategy adopted by SOLPS-ITER for molecular ions, questioning the validity of the static approximation under the operating conditions typical of LPDs. This issue is especially relevant given that SOLPS-ITER is one of the most widely used and well-established codes in magnetic confinement fusion research. Comparative analyses with 0D models provide an effective means of addressing this problem, as the two approaches are highly complementary and can be employed in an integrated manner.

As discussed in Subsection 2.3.5, an open issue in the global modeling of hydrogen plasmas concerns the limited extension of existing models to isotopic variants and the accurate treatment of isotope-dependent effects. In the literature, global models have indeed been applied to deuterium plasmas; however, these typically consist of hydrogen models applied directly to deuterium systems, without explicitly accounting for the isotopic difference. As a result, the implemented physics and chemistry, including the cross sections, remain those of hydrogen, and isotopic effects are neglected. Among these, vibrational levels differ between the two isotopes in both number and energy, as do the associated cross sections.

The present thesis addresses these issues through three main objectives. The first is the development and benchmarking of a global model for hydrogenic plasmas that explicitly accounts for deuterium, addressing the gap identified above. The second is the investigation of deuterium plasmas in the GyM LPD by means of this model, with the additional aim of validating its predictions against experimental observations. The third is the assessment of the validity of the molecular-ion modeling strategy adopted in SOLPS-ITER

for LPD simulations, with particular attention to GyM, where its validity has already been questioned. This last activity represents the in-depth study carried out as part of the *Honours Programme* in "Scientific Research in Industrial Engineering - Nuclear Science and Technology", attended during the Master's degree at Politecnico di Milano.

The following chapters present this work in detail. The global model is first developed for pure hydrogen plasmas, enabling direct benchmarking against existing models in the literature, and is subsequently extended to deuterium through a dedicated treatment of the relevant isotopic effects. It is then applied to the GyM linear plasma device, where its predictions are validated against experimental measurements. In addition, the model is used to analyze the plasma, providing estimates of quantities that are not directly accessible experimentally, such as the absorbed power fraction and the plasma composition. Finally, simulations of GyM under representative operating conditions are performed using SOLPS-ITER. The predicted electron density, electron temperature, and plasma composition are compared with the corresponding results obtained from the global model, the main differences between the two approaches are identified, and the implications of the static approximation adopted in SOLPS-ITER are assessed.

3 | Development of a global model for Hydrogen and Deuterium plasmas

A global model for hydrogenic plasmas has been developed and implemented in a Python code, including both hydrogen and deuterium species. The model is intended for low-temperature ($\lesssim 20$ eV) and low-to-intermediate pressure (from $\sim 10^{-2}$ to ~ 15 Pa) plasmas sustained by electron heating. Under these conditions, electron and ion populations are weakly coupled, such that $T_e \gg T_i \approx T_g$. Consequently, the ion and neutral power balance equations are neglected, and their temperatures are assumed to remain constant. The model consists of a system of coupled non-linear differential equations comprising one particle balance equation for each plasma species (excluding electrons), a charge balance equation for the electron density, and an electron power balance equation.

The development started from a hydrogen plasma model based on reference literature works, such as those by Hjartarson *et al.* [56] and Samuell and Corr [47]. The modeling approaches adopted for the different terms described in Section 2.3 were selected and implemented on the basis of physically justified assumptions. Whenever available, updated cross-section data were employed, and specific adaptations were introduced to account for the considered geometry. In addition, magnetic confinement effects were incorporated through dedicated corrections to the wall-loss terms.

The model was subsequently extended to deuterium plasmas through the development of a dedicated reaction database. Compared with hydrogen, the availability of data, reaction rates, and cross sections for deuterium is significantly more limited. For this reason, the deuterium database was constructed by applying reasonable physical assumptions and approximations whenever dedicated data were unavailable. A detailed description of the implemented reactions and corresponding source data is provided in Section 3.1, with particular focus on hydrogen in Subsection 3.1.1 and on deuterium in Subsection 3.1.2.

The final form of the model is summarized in Section 3.2, where the governing equations,

solution procedure, and available modeling options are reported explicitly.

Finally, Section 3.3 presents the benchmark and validation activities carried out on hydrogen plasmas. The three systems selected for this purpose, together with the results of the comparison with the developed model, are described in Subsections 3.3.1, 3.3.2, and 3.3.3. Additional observations and considerations regarding the hydrogen plasma simulations are reported in Subsection 3.3.4.

3.1. Included species and reactions

In this section, the chemistry included in the model is described in detail. For hydrogen plasmas, the set of modeled species consists of atomic, H, and molecular hydrogen, H₂, including its lowest vibrational levels, H₂($\nu = 1-14$), the positive atomic and molecular ions H⁺, H₂⁺, and H₃⁺, the negative ion H⁻, and electrons, e⁻. For deuterium plasmas, the corresponding species are included, with 20 vibrational levels considered instead of 14.

A summary of all physical processes and reactions included in the model is presented in Figure 3.1. For computational convenience, particle exchange with the external environment and plasma-wall interaction processes are treated as effective reactions, in addition to the volumetric ones. The procedures adopted to evaluate the corresponding rate coefficients and reaction rates are described in the following, and summarized in Table 3.1. Volumetric reactions are not discussed here, as they are specific to the plasma isotope considered (hydrogen or deuterium) and are therefore presented separately in the dedicated sections below.

External particle exchange terms are of two kind, gas feeding and pumping. For the gas feeding, the inlet flow rate Γ_{feed} , in s⁻¹, is typically fixed by the user as an input parameters. The feed species is the molecular neutral, and the reaction rate is simply computed as $S_{feed} = \Gamma_{feed}/V$ in m⁻³s⁻¹, with V the volume of the system.

For gas pumping instead, it is considered a system in which the pumps acts to keep the internal pressure at a fixed imposed value. The pumped species include all neutral and positively charged species. Negative ions, by contrast, are assumed to be confined within the plasma bulk by the positive plasma potential (as discussed in Subsection 2.3.4), preventing them from efficiently reaching the walls; consequently, they are not included in the pumping term. In specific cases in which the pumps are in a position not directly reached by the ionized portion of the gas, then only the neutral species are accounted to

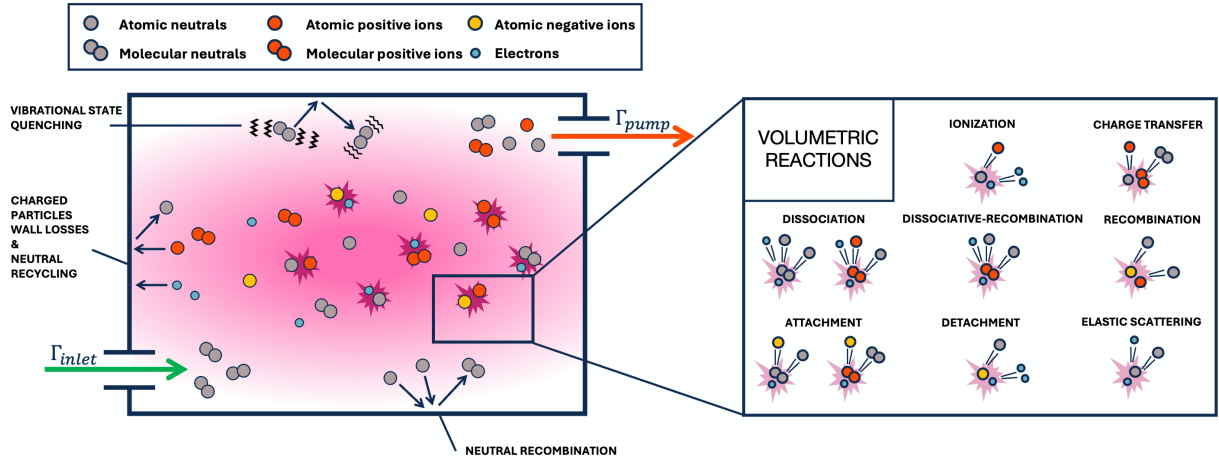


Figure 3.1: Summary of the physical processes and reactions included in the hydrogenic plasma model.

be removed. The pumping rate for the a -th specie can be expressed as [47]:

$$S_{a,pump} = n_a \frac{\Gamma_{feed}}{V n_{gas,initial}} \quad (3.1)$$

where n_a is the density of the considered specie in m^{-3} , and $n_{gas,initial}$ is the initial particle density of the gas before the formation of the plasma, calculated using the *ideal gas law* at the specified gas temperature and pressure, which are imposed as input parameters.

For what concerns wall losses for charged species, the effective area, A_{eff} is computed according to the pressure regime. As discussed in Subsection 2.3.3, in the low-pressure regime, $\lambda_i \gtrsim (R, L)$, for an electropositive plasma, $A_{eff} \approx 0.5A$ [41]. Applying a correction for the electronegativity effects, introduced in Subsection 2.3.4, it can be written as:

$$A_{eff} \approx \frac{0.5A}{1 + \alpha_0} \quad (3.2)$$

For intermediate pressure regime, $(R, L) \gtrsim \lambda_i \gtrsim (T_i/T_e)(R, L)$, the same approach as Samuelli and Corr [47] has been applied, using the edge-to-center density ratios described by equations (2.58) to (2.61). The formulation has been extended also to account for parallelepiped geometries with dimensions L_x , L_y and L_z :

$$A_{eff} = 2(L_x L_y h_z + L_y L_z h_x + L_z L_x h_y) \quad (3.3)$$

$$h_{(L_x, L_y, L_z),a} = h_{l,a} \quad h_{(x,y,z)}^2 = h_{(L_x, L_y, L_z),a}^2 + h_c^2 \quad (3.4)$$

In the case of magnetic confinement, the ion losses in the confined direction have been evaluated as done by Tonello *et al.* [50] and reported in equation (2.48).

For atomic neutral recombination at the wall and vibrational quenching the rate coefficient expressed by equation (2.53) has been used, with quenching probability $\gamma_Q = 1$.

Table 3.1: Surface reactions included in the developed model, valid for both hydrogen and deuterium.

ID	Reaction	Reactivity [s ⁻¹]
Ion-wall losses and recombination		
S.1	$H^+ + wall \rightarrow H$	$u_{B,H} + \frac{A_{eff}}{V}$
S.2	$H_2^+ + wall \rightarrow 2H$	$u_{B,H_2^+} + \frac{A_{eff}}{V}$
S.3	$H_3^+ + wall \rightarrow 2H + H$	$u_{B,H_3^+} + \frac{A_{eff}}{V}$
S.4	$H^+, H_2^+, H_3^+ \rightarrow confinement\ escape$	$\frac{D_{\perp}}{\lambda_n} \frac{A_{\perp}}{V}$
Neutral-wall recombination		
S.5	$H + H + wall \rightarrow H_2$	$\left[\frac{\Lambda_0^2}{D_H} + \frac{2V(2 - \gamma_r)}{A\bar{v}_H \gamma_r} \right]^{-1}$
Vibrational state quenching		
S.6	$H_2(X^1\Sigma_g^+, v) + wall \rightarrow H_2(X^1\Sigma_g^+, v-1)$	$\left[\frac{\Lambda_0^2}{D_{H_2}} + \frac{2V(2 - \gamma_Q)}{A\bar{v}_{H_2} \gamma_Q} \right]^{-1}$
Gas feeding		
S.7	$H_2 \rightarrow enters\ the\ plasma$	Γ_{feed}
Gas Pumping		
S.8	$H, H_2, H^+, H_2^+, H_3^+ \rightarrow exit\ the\ plasma$	$\frac{\Gamma_{feed}}{V n_{gas, initial}}$

3.1.1. Hydrogen database

In this section, the complete set of volumetric reactions included in the hydrogen model is reported along with the cross sections or reactivity sources. Table 3.2 lists the reactions involving only the ground states of the considered species, whereas Table 3.3 reports those involving the lowest 14 vibrational levels of the electronic ground state of H₂. In some cases, reactivity coefficients were directly available in the literature; otherwise, they were calculated from the corresponding cross sections assuming a Maxwell-Boltzmann distribution, as described by Equations 2.32 and 2.33.

Particle collisions can be classified into two main categories: elastic and inelastic. The latter includes both excitation of internal degrees of freedom and a wide range of chemical and physical reactions. Among these, ionization is the fundamental mechanism responsible for plasma formation. Electron attachment, on the other hand, leads to the production of negative ions, which are subsequently destroyed through detachment processes or recombination with positive ions. Charge-transfer reactions play a crucial role in hydrogen

plasmas, as they represent the primary formation pathway of H_3^+ . Additional processes included in the model are molecular dissociation, dissociative recombination of positive ions with electrons, and associative ionization.

Table 3.2: Hydrogen volumetric reactions included in the model for ground-state species.

ID	Reaction	Ref.	ID	Reaction	Ref.
	Elastic scattering				
H.1	$e^- + H_2 \rightarrow e^- + H_2$	[96, 97]	H.11	$e^- + H_2^+ \rightarrow H + H^+ + e^-$	[56, 104]
H.2	$e^- + H \rightarrow e^- + H$	[98]	H.12	$e^- + H_3^+ \rightarrow 2H + H^+ + e^-$	[56, 100]
	Ionization			Dissociative recombination	
H.3	$e^- + H_2 \rightarrow 2e^- + H_2^+$	[96, 97]	H.13	$e^- + H_2^+ \rightarrow 2H$	[56, 104]
H.4	$e^- + H \rightarrow 2e^- + H^+$	[98]	H.14	$e^- + H_3^+ \rightarrow 3H$	[56, 104]
	Attachment		H.15	$e^- + H_3^+ \rightarrow H + H_2$	[56, 104]
H.5	$e^- + H_2 \rightarrow H^- + H$	[99]		Recombination	
H.6	$e^- + H_3^+ \rightarrow H_2^+ + H^-$	[56, 100]	H.16	$H + H^- \rightarrow H_2 + e$	[105]
	Detachment		H.17	$H^+ + H^- \rightarrow 2H$	[56, 106]
H.7	$e^- + H^- \rightarrow H + 2e^-$	[56, 101]	H.18	$H^+ + H^- \rightarrow H + H(n = 2, 3)$	[105]
	Charge transfer		H.19	$H_2^+ + H^- \rightarrow 3H$	[56, 106]
H.8	$H + H_2^+ \rightarrow H_2 + H^+$	[102]	H.20	$H_2^+ + H^- \rightarrow H_2 + H$	[105]
H.9	$H_2 + H_2^+ \rightarrow H + H_3^+$	[102]	H.21	$H_3^+ + H^- \rightarrow 4H$	[56, 106]
	Dissociation		H.22	$H_3^+ + H^- \rightarrow H_2 + H_2$	[105]
H.10	$e^- + H_2 \rightarrow 2H + e^-$	[56, 103]		Associative ionization	
			H.23	$H_2 + H \rightarrow H_3^+ + h\nu$	[56, 107]

Table 3.3: Hydrogen volumetric reactions included in the model involving vibrationally excited states.

ID	Reaction	Ref.
	Excitation	
H.24	$e^- + H_2(X^1\Sigma_g^+; \nu) \rightarrow e^- + H_2(X^1\Sigma_g^+; \nu') + h\nu$	$(\nu, \nu' = 0 - 14)$ [108, 109]
	Ionization	
H.25	$e^- + H_2(X^1\Sigma_g^+; \nu) \rightarrow 2e^- + H_2^+$	$(\nu = 1 - 14)$ [108, 110]
	Ionizing dissociation	
H.26	$e^- + H_2(X^1\Sigma_g^+; \nu) \rightarrow 2e^- + H^+ + H$	$(\nu = 0 - 14)$ [95, 111]
	Attachment	
H.27	$e^- + H_2(X^1\Sigma_g^+; \nu) \rightarrow H^- + H$	$(\nu = 1 - 14)$ [95, 111]
	Dissociation	
H.28	$e^- + H_2(X^1\Sigma_g^+; \nu) \rightarrow e^- + 2H$	$(\nu = 1 - 14)$ [108, 112]

The inclusion of reactions involving vibrationally excited molecules is of fundamental importance. Power losses associated with molecular excitation by electron impact constitute a significant contribution to the overall energy balance and must therefore be properly accounted for. Vibrational excitation and de-excitation processes are included for all possible pairs of vibrational levels $\nu, \nu' = 0 - 14$. Ionization, dissociation, and electron

attachment are considered for vibrational levels $\nu = 1 - 14$, while ionizing dissociation is included for all vibrational states, including the ground state.

Cross sections for vibrational excitation and de-excitation, ionization, and dissociation are taken from the *MCCC Database* [108], which provides a comprehensive set of theoretically calculated data validated against established experimental and theoretical studies. For ionizing dissociation and electron attachment, the data reported by Janev *et al.* [111] have been adopted. These are the same data included in the HYDEL database [95] currently used by SOLPS-ITER.

3.1.2. Deuterium database

In this section, the complete set of reactions and data employed for deuterium simulations is presented. The main challenges associated with the isotopic adaptation of the model emerge clearly in this context. On one hand, the availability of reaction data for deuterium is considerably more limited than for hydrogen, making it difficult to identify dedicated datasets for all the reactions included in the hydrogen model. On the other hand, hydrogen reaction data cannot be directly transposed to its isotope without careful assessment.

Table 3.4: Deuterium volumetric reactions included in the model for ground-state species.

ID	Reaction	Ref.	ID	Reaction	Ref.
Elastic scattering			Dissociation		
D.1	$e^- + D_2 \rightarrow e^- + D_2$	[113, 114]	D.11	$e^- + D_2 \rightarrow 2D + e^-$	[56, 103]*
D.2	$e^- + D \rightarrow e^- + D$	[98]*	D.12	$e^- + D_2^+ \rightarrow D + D^+ + e^-$	[56, 104]*
Ionization			D.13	$e^- + D_3^+ \rightarrow 2D + D^+ + e^-$	[56, 100]*
D.3	$e^- + D_2 \rightarrow 2e^- + D_2^+$	[113, 114]	Dissociative recombination		
D.4	$e^- + D \rightarrow 2e^- + D^+$	[98]*	D.14	$e^- + D_2^+ \rightarrow 2D$	[56, 104]*
D.5	$e^- + D_2 \rightarrow 2e^- + D^+ + D$	[95, 111]*	D.15	$e^- + D_3^+ \rightarrow 3D$	[56, 104]*
Attachment			D.16	$e^- + D_3^+ \rightarrow D + D_2$	[56, 104]*
D.6	$e^- + D_2 \rightarrow D^- + D$	[113, 114]	Recombination		
D.7	$e^- + D_3^+ \rightarrow D_2^+ + D^-$	[56, 100]**	D.17	$D^+ + D^- \rightarrow 2D$	[115]
Detachment			D.18	$D_2^+ + D^- \rightarrow 3D$	[115]
D.8	$e^- + D^- \rightarrow D + 2e^-$	[56, 101]**	D.19	$D_2^+ + D^- \rightarrow D_2 + D$	[115]
Charge transfer			D.20	$D_3^+ + D^- \rightarrow 4D$	[115]
D.9	$D + D_2^+ \rightarrow D_2 + D^+$	[102]	D.21	$D_3^+ + D^- \rightarrow D_2 + D_2$	[115]
D.10	$D_2 + D_2^+ \rightarrow D + D_3^+$	[102]			

(*) Cross section adopted from hydrogen, assumed to be a reasonable approximation.

(**) Cross section adopted from hydrogen due to the lack of isotope-specific data, but its validity is considered uncertain.

Table 3.5: Deuterium volumetric reactions included in the model involving vibrationally excited states.

ID	Reaction	Ref.
Excitation		
D.23	$e^- + D_2(X^1\Sigma_g^+; \nu) \rightarrow e^- + D_2(X^1\Sigma_g^+; \nu') + h\nu$	$(\nu, \nu' = 0 - 20)$ [108, 109]
Ionization		
D.24	$e^- + D_2(X^1\Sigma_g^+; \nu) \rightarrow 2e^- + D_2^+$	$(\nu = 1 - 20)$ [108, 110]
Attachment		
D.25	$e^- + D_2(X^1\Sigma_g^+; \nu) \rightarrow D^- + D$	$(\nu = 1 - 20)$ [76, 116]
Dissociation		
D.26	$e^- + D_2(X^1\Sigma_g^+; \nu) \rightarrow e^- + 2D$	$(\nu = 1 - 20)$ [76, 116]

The change in nuclear mass has several consequences for the overall plasma dynamics. First, it affects quantities such as the Bohm velocity ($u_{B,i} = \sqrt{eT_e/m_i}$) and the energy exchanged during elastic collisions ($E_{R,el} \simeq 3eT_em_e/m_i$). However, both of them are computed self-consistently within the model. The main challenge concerns the quantities provided as external inputs, namely the cross sections and the reaction rate coefficients. In this respect, the isotopic mass change has two principal effects: the modification of the reduced mass (i.e., $m_1m_2/(m_1 + m_2)$ for two colliding particles) and the variation in the energies and number of excited states.

The variation in the reduced mass alters the relative velocity corresponding to a given relative kinetic energy and may therefore affect the shape of velocity or energy dependent cross sections. This effect is significant mainly for heavy-particle collisions involving atoms and molecules. In electron-impact collisions, by contrast, the large mass difference between electrons and heavy particles makes the change in reduced mass negligible. It is therefore reasonable to assume that the corresponding cross sections and reaction rate coefficients do not vary significantly between hydrogen and deuterium. To support this assumption, Figure 3.2 compares different reactions for which both hydrogen and deuterium cross-section data are available. It can be observed that, in most cases, the cross sections are nearly identical, with the notable exception of electron attachment processes, where electron-affinity effects become important. Consequently, dedicated deuterium cross sections were employed whenever available, while hydrogen data were adopted for the remaining electron-impact reactions.

In collisions involving atoms and molecules, however, this assumption is no longer valid, and dedicated data should be always used. For recombination reactions, suitable deu-

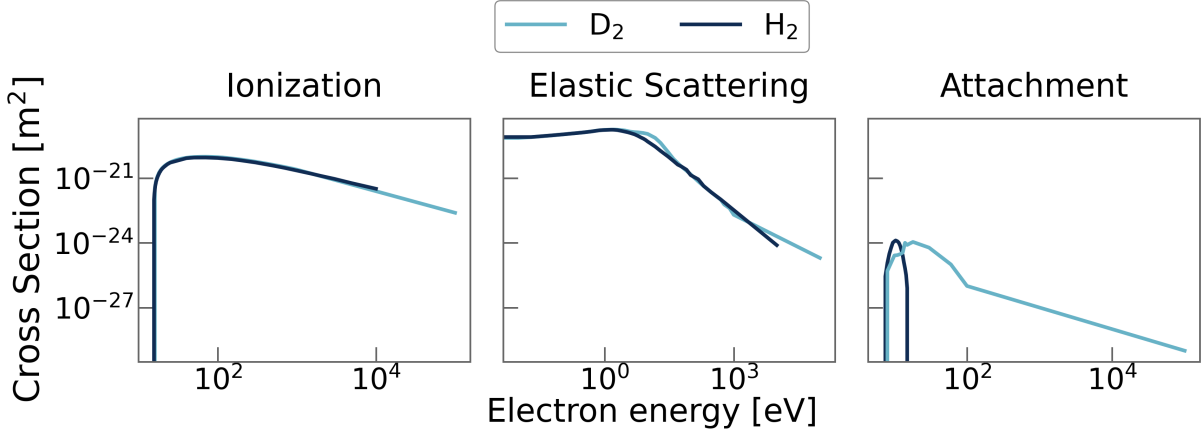


Figure 3.2: Hydrogen and deuterium cross section comparison, data from LXCat Database [117].

terium data could not be identified, and the approximate scaling law proposed by Hickman [115] was adopted.

The variation in the vibrational energy levels represents a further complication. Since the vibrational structure of deuterium differs from that of hydrogen, dedicated cross sections are required and hydrogen data cannot be directly applied. For this reason, only deuterium-specific datasets were employed for reactions involving vibrationally excited states. This is also the reason why only 20 vibrational levels were included in the model, even though 21 levels exist for deuterium: the necessary data for the highest vibrational state were not available.

The final set of reactions together with the cross section and reactivity references, is reported in Tables 3.4 and 3.5.

3.2. Model summary

A complete summary of the implemented model is provided in this section.

The model takes as input the system geometry, the boundary condition types and their corresponding parameters (e.g., $D_{\perp}$, γ , etc.), the inlet gas flow rate Γ_{feed} , the input power density P_{input} , and the initial neutral gas state, defined by its temperature T_g and pressure p . Starting from these initial conditions, the code evolves the system in time, leading to plasma formation.

The governing equations are presented below together with the corresponding notation, whose definitions are listed in Table 3.6.

Model equations

$$\left\{ \begin{array}{ll} \frac{dn_a}{dt} = \sum_R S_{a,R} & \text{particle balance} \\ n_e = \sum_a \frac{n_a q_a}{e} & \text{charge balance} \\ \frac{3}{2} en_e \frac{dT_e}{dt} = P_{input}^e - P_{coll,loss}^e - P_{wall,loss}^e - \frac{3}{2} e T_e \sum_R S_{e,R} & \text{power balance} \end{array} \right. \quad (3.5)$$

Collisional power losses

$$\left\{ \begin{array}{l} P_{coll,loss}^e = en_e \sum_X n^{(X)} \epsilon_c^{(X)} k_{iz}^{(X)} \\ \epsilon_c^{(X)} = \epsilon_{iz}^{(X)} + \sum_j \epsilon_{ex,j}^{(X)} \frac{k_{ex,j}^{(X)}}{k_{iz}^{(X)}} + \frac{k_{el}^{(X)}}{k_{iz}^{(X)}} \frac{3m_e}{m^{(X)}} T_e \end{array} \right. \quad (3.6)$$

Wall power losses

$$\left\{ \begin{array}{ll} P_{wall,loss}^e = eu_B n_i \frac{A_{eff}}{V} (2T_e + |V_{sf}| + |V_{pre-sheath}|) & \text{unconfined direction} \\ P_{wall,loss}^e = \frac{3}{2} e T_e n_i \frac{D_{\perp}}{\lambda_n} \frac{A_{\perp}}{V} & \text{confined direction} \end{array} \right. \quad (3.7)$$

In the particle balance equations, the reaction source terms include all the processes described in the previous section, and are computed according to Equation 2.31. The subscript a refers to all the included species except electrons.

The last term in the power balance equation accounts for the energy loss associated with the net generation of electrons. Newly created electrons do not generally possess the mean energy of the remaining population, T_e , and must be thermalized through collisions with the background electrons. The energy required for this thermalization process represents an effective loss term. This contribution was not included in the reference model of Samuelli and Corr [47], but has been incorporated here following similar treatments reported in the literature [43, 50].

The collisional energy losses per electron-ion pair created are reported in Figure 3.3. The results obtained for hydrogen are compared with the literature values reported by Samuelli and Corr [47] and Yang *et al.* [59], showing overall good agreement, as illustrated in Figure 3.4.

The model can accommodate both cylindrical and parallelepiped geometries, including

Table 3.6: List of symbols of the developed model.

Symbol	Unit	Description
A_{eff}	m^2	Effective area for ion wall losses
$A_{\perp}$	m^2	Surface in the confinement direction
$D_{\perp}$	$\text{m}^2 \text{s}^{-1}$	Anomalous diffusion coefficient
$k_{\text{el}}^{(X)}$	$\text{m}^3 \text{s}^{-1}$	Elastic scattering rate coefficient for the neutral species X with electrons
$k_{\text{ex},j}^{(X)}$	$\text{m}^3 \text{s}^{-1}$	Excitation rate coefficient for the neutral species X in the j final state
$k_{\text{iz}}^{(X)}$	$\text{m}^3 \text{s}^{-1}$	Ionization rate coefficient for the neutral species X
m_e	kg	Electron mass
$m^{(X)}$	kg	Mass of the neutral species X
n_a	m^{-3}	Particle density of the a -th species
n_e	m^{-3}	Electron density
n_i	m^{-3}	Ion density
$n^{(X)}$	m^{-3}	Particle density of the neutral species X
P_{input}^e	W m^{-3}	Input power density
$P_{\text{coll,loss}}^e$	W m^{-3}	Collisional power density losses
$P_{\text{wall,loss}}^e$	W m^{-3}	Wall power density losses
q_a	C	Charge of species a
$S_{a,R}$	$\text{m}^{-3} \text{s}^{-1}$	Source rate of a -particles due to reaction R
$S_{e,R}$	$\text{m}^{-3} \text{s}^{-1}$	Source rate of electrons due to reaction R
T_e	eV	Electron temperature
u_B	m s^{-1}	Ion Bohm velocity
V	m^3	Plasma volume
V_{sf}	eV	Potential drop in the sheath
$V_{\text{pre-sheath}}$	eV	Potential drop in the pre-sheath
$\epsilon_c^{(X)}$	eV	Collisional energy loss per electron-ion pair created in the collision with the neutral species X
$\epsilon_{\text{ex},j}^{(X)}$	eV	Excitation energy of the neutral species X in the j final state
$\epsilon_{\text{iz}}^{(X)}$	eV	Ionization energy of the neutral species X
λ_n	m	Density decay length

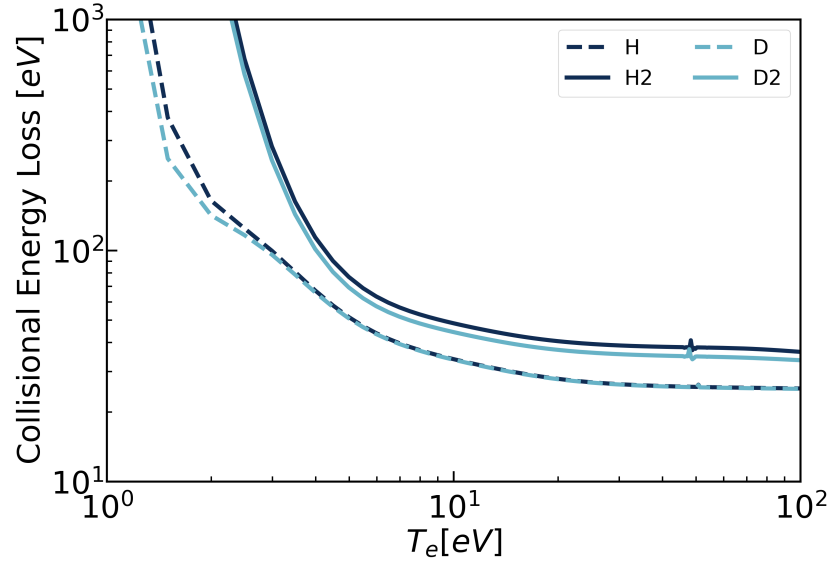


Figure 3.3: Collisional energy loss per electron ion-pair created. Comparison among the computed curves for H, H₂, D and D₂.

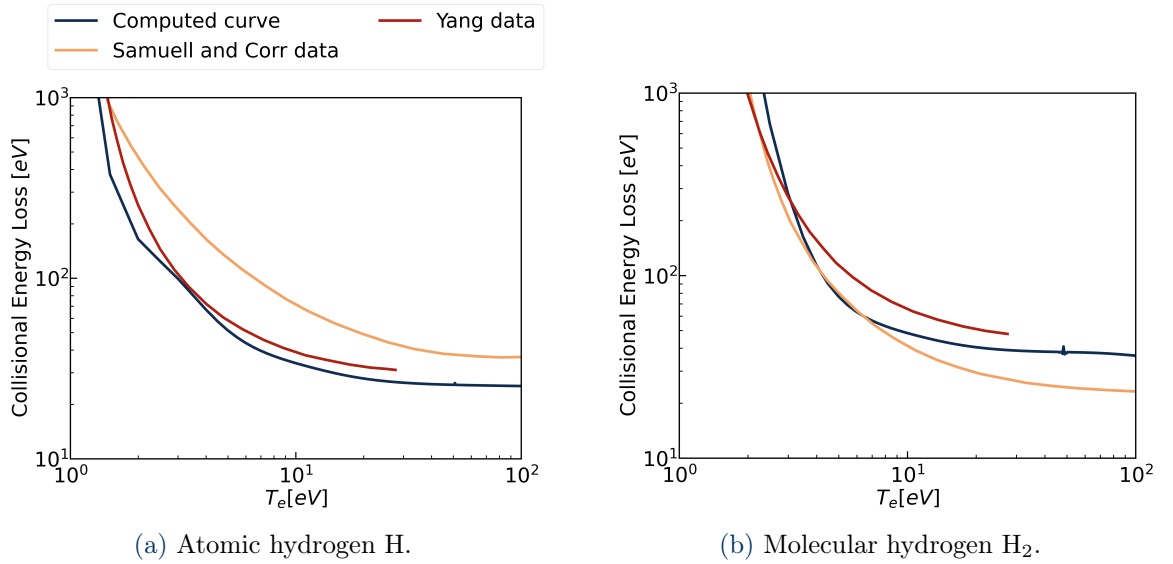


Figure 3.4: Collisional energy loss per electron ion-pair created. Comparison among the computed curves for H and H₂, and the literature data of Samuel and Corr [47] and Yang *et al.* [59].

the possibility of specifying open boundaries. Furthermore, distinct volumes may be assigned to the plasma and neutral gas regions when required, enabling the construction of combined geometrical configurations.

The resulting system of equations is numerically integrated in time using a fifth-order implicit Runge-Kutta scheme¹. To improve numerical convergence, the state vector, comprising the species densities and the electron temperature, is normalized over user-defined reference values, thereby bringing all variables to comparable orders of magnitude.

3.3. Benchmark and validation

The validity of the developed model was assessed through benchmarking against existing models, while simultaneously validating the results against the experimental data reported in the corresponding studies. Owing to the lack of dedicated deuterium plasma models available in the literature, the benchmarking activity was carried out using hydrogen plasmas only.

The selection of the reference studies was based on three main criteria. First, the modeled plasma had to consist exclusively of hydrogen species. Second, the included species, underlying physics and range of operating conditions had to be comparable to those considered in the developed model. Finally, the model had to be adaptable to the geometry of the selected experimental systems.

Based on these criteria, two studies were considered. The first is the work by Samuel and Corr (2016) [47], which served as the primary reference throughout the development process. The authors validated their model against a *Gaseous Electronics Conference (GEC) reference cell* [71] and subsequently applied it to the *MAGPIE* reactor [72]. In the present work, both systems were modeled and used for benchmarking. The corresponding results are presented in Subsections 3.3.1 and 3.3.2.

The second study is that of Yang *et al.* (2018) [59], who benchmarked and validated their *Global Model for Negative Hydrogen Ion Source (GMNHIS)*. Their work first compared the GMNHIS with the existing *Global Enhanced Vibrational Kinetic Model (GEVKM)* [73] and subsequently validated the model against measurements from an *Electron Cyclotron Resonance (ECR) discharge*. The latter system was considered in the present work and is discussed in Subsection 3.3.3.

¹In the Python implementation, this is performed using the `solve_ivp` function with the *Radau* method.

3.3.1. Gaseous Electronic Conference reference cell

The Gaseous Electronic Conference (GEC) reference cell is a standardized experimental device designed to be reproduced identically in different laboratories, enabling direct comparison of measurements and results. Being a well-characterized system, it represents an attractive choice for model benchmarking and validation.

The original design consists of two water-cooled aluminum electrodes, each with a diameter of 10 cm, arranged in a parallel-plate configuration and equipped with a showerhead gas inlet. The reactor was originally intended to operate in capacitively coupled mode. Subsequently, some researchers retrofitted the upper electrode with an inductively coupled coil, allowing the generation of higher-density plasmas while independently controlling the sheath DC bias through a capacitively coupled RF source [71].

The experimental data used for validation were taken from the PhD thesis of Kadetov [118], who performed an extensive characterization of a modified GEC reference cell. The reactor was operated in inductively coupled mode, and plasma parameters were measured using a Langmuir probe over a range of operating pressures and input powers.

In the work of Samuelli and Corr [47], the reactor radius is assumed to be 80 mm, corresponding to the radius of the lower electrode, while the reactor length is taken as 50 mm, corresponding to the distance between the upper quartz plate and the lower metallic electrode. The wall recombination probability for atomic neutrals, γ_r , is set to 0.05 in order to account for the combination of metallic and quartz surfaces present in the reactor.

For comparison with their model, Samuelli and Corr selected data corresponding to a pressure scan from 0.67 to 12 Pa at a constant input power of 300 W, and a power scan from 100 to 1200 W at a constant pressure of 10 Pa. The inlet gas flow rate was assumed to be 100 sccm while the neutral gas temperature was estimated using the empirical correlation $T_g = 300(1 + 1.5P)$, where T_g is expressed in K and P is the input power in kW. The ion temperature was determined using a pressure-dependent correlation. For pressures below 1 mTorr, a constant value of $T_i = 0.5$ eV was assumed. For higher pressures, the expression $T_i = (0.5 - T_g)/p + T_g$ was used, where both T_i and T_g are expressed in eV, and p is the pressure in mTorr.

The model developed in this work was used to perform simulations under the same assumptions and operating conditions adopted by Samuelli and Corr. The resulting electron densities and electron temperatures for both parameter scans are shown in Figure 3.5, together with the predictions of the reference model and the corresponding experimental measurements.

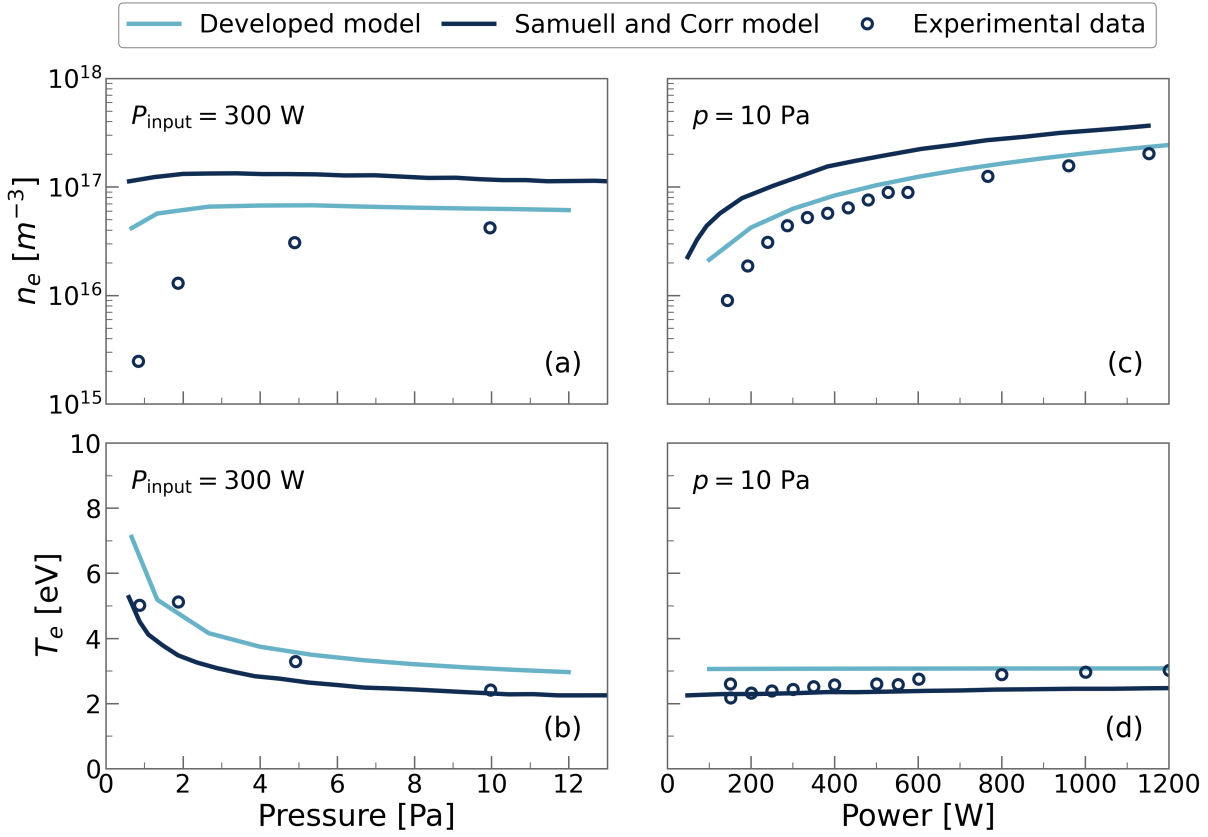


Figure 3.5: Comparison between the developed model, the model of Samuel and Corr [47], and the experimental measurements reported in their work for the GEC reference cell. (a) Electron density and (b) electron temperature as functions of gas pressure at constant input power, $P_{\text{input}} = 300$ W; (c) electron density and (d) electron temperature as functions of input power at constant pressure, $p = 10$ Pa.

The qualitative trends of both electron density and electron temperature are in good agreement with those predicted by the reference model for both scans. From a quantitative perspective, the electron densities obtained with the developed global model exhibit closer agreement with the experimental data. For the electron temperature, both models show a comparable level of agreement with the experimental measurements, and no clear conclusion can be drawn regarding the relative performance of the two models.

3.3.2. MAGPIE Reactor

The *Magnetized Plasma Interaction Experiment MAGPIE* is a low-pressure, magnetically enhanced helicon² reactor located at the Australian National University [72]. The reactor launches helicon waves into a region of increasing magnetic field strength, generating a high-density plasma downstream of the source region. The facility is used to investigate fundamental plasma phenomena, plasma-material interactions under extreme conditions, and to serve as a test bed for the development of diagnostics for the edge regions of fusion reactors [72].

The source region consists of a 1 m long tube with an inner diameter of 9.8 cm. One end of the tube is connected to a 68 cm long stainless-steel target chamber, while the other is connected to a steel T-piece leading to the pumping system. Power can be supplied either at a frequency of 13.56 MHz up to 5 kW or at 7 MHz up to 20 kW. A DC magnetic field is generated by two sets of solenoids, typically configured to produce a converging magnetic-field topology.

Due to its low aspect ratio (i.e., a small R/L ratio), MAGPIE presents a significant challenge for zero-dimensional modeling. In compact plasma systems, the electron mean free path is often larger than the characteristic dimensions of the device; however, this assumption does not necessarily hold in elongated systems, where spatial homogeneity cannot be assumed *a priori*. Furthermore, the presence of strong magnetic fields suppresses radial diffusion, making the determination of the effective plasma volume uncertain [47].

In the work of Samuelli and Corr [47], the plasma was assumed to have a length of 1 m, corresponding to the discharge length when a sample holder is installed, and a radius equal to the physical tube radius of 9.8 cm. This approximation is considered valid for low to moderate magnetic-field strengths, for which the plasma remains in the weakly magnetized regime. The wall recombination probability was set to $\gamma_r = 0.05$, the gas temperature was fixed at $T_g = 600$ K, and the inlet flow rate was 50 sccm.

For the comparison between their model predictions and the experimental measurements, Samuelli and Corr considered two datasets: a pressure scan from 0.40 to 1.33 Pa at a constant input power of $P_{\text{input}} = 1.5$ kW, and a power scan from 200 to 1000 W at a constant pressure of 1.33 Pa.

The model developed in this work was used to perform simulations under the same assumptions and operating conditions adopted by Samuelli and Corr. The resulting electron

²Helicon waves are bounded electromagnetic waves in magnetized plasmas with frequencies between the ion cyclotron frequency and the electron cyclotron frequency. They are of considerable interest because they can propagate at much higher plasma densities than many other wave modes.

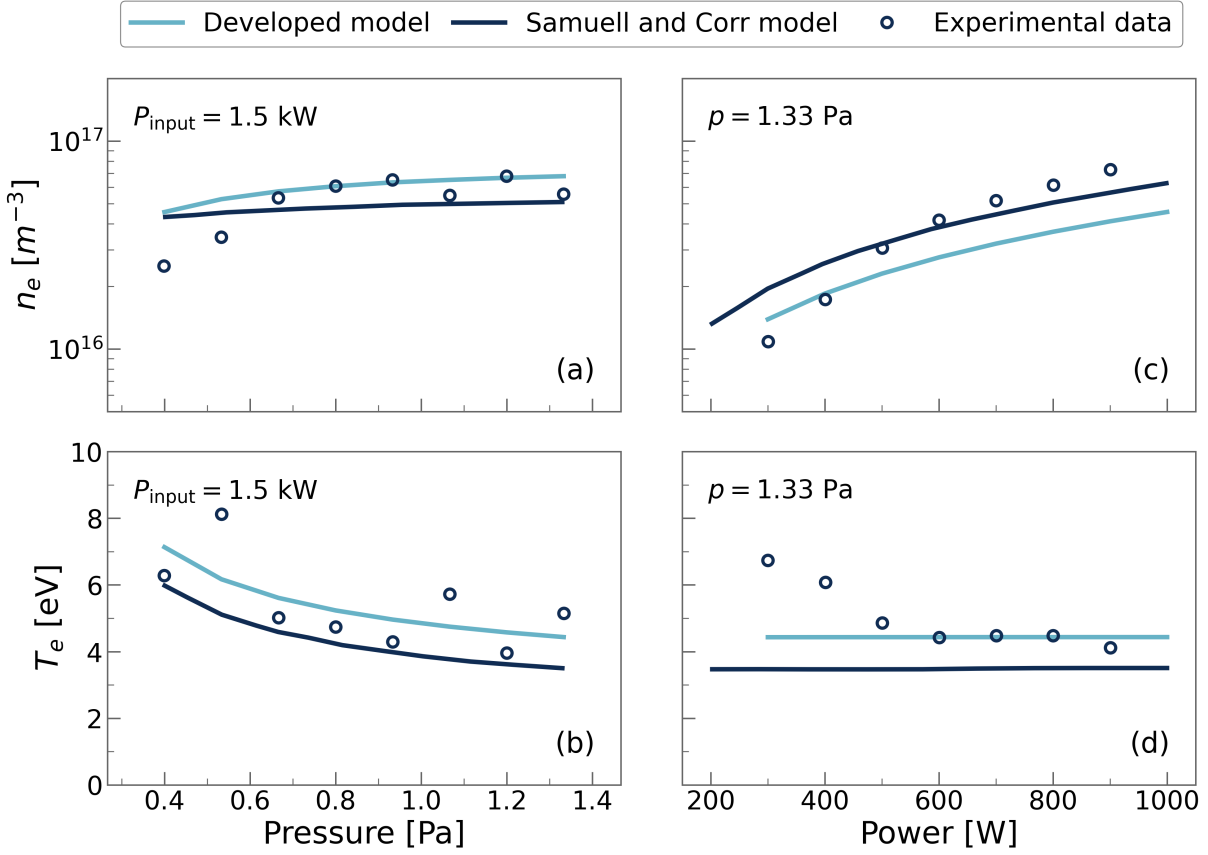


Figure 3.6: Comparison between the developed model, the model of Samuelli and Corr [47], and the experimental measurements reported in their work for the MAGPIE reactor. (a) Electron density and (b) electron temperature as functions of gas pressure at constant input power, $P_{\text{input}} = 1.5$ kW; (c) electron density and (d) electron temperature as functions of input power at constant pressure, $p = 1.33$ Pa.

densities and electron temperatures for both parameter scans are shown in Figure 3.6, together with the predictions of the reference model and the corresponding experimental measurements.

The qualitative trends of both electron density and electron temperature are in good agreement with those predicted by the reference model for both scans. From a quantitative perspective, the electron temperatures obtained with the developed global model exhibit closer agreement with the experimental data. Regarding electron density, in the pressure scan both models show a comparable level of agreement with the experimental measurements, and no clear conclusion can be drawn regarding their relative performance. In the power scan, however, the developed model underestimates the electron density with respect to both the reference model and the experimental data, while still remaining in close proximity; this level of agreement is nevertheless acceptable for a global model.

3.3.3. Electron Cyclotron Resonance Discharge

The ECR discharge considered in the work of Yang *et al.* [58] is generated in the negative ion source Prometheus I [119]. The device consists of a cubic stainless-steel chamber with a side length of 24 cm, in which the plasma is sustained by a two-dimensional array of elementary ECR sources. Each source is powered by an independent solid-state microwave generator operating at 2.45 GHz and delivering up to 180 W. An impedance-matching tuner integrated into each source maximizes the microwave power absorbed by the plasma. The chamber is evacuated by a turbomolecular pump mounted on the bottom flange, allowing a base pressure of $1.3332 \cdot 10^{-5}$ Pa to be reached.

The experimental data used for comparison with the model were obtained under the following operating conditions. Pure H_2 was fed into the source at flow rates ranging from 2.1 to 23.2 sccm. The working pressure was varied between 0.133 and 2.67 Pa while maintaining a constant absorbed power of 900 W. Plasma parameters were measured using a cylindrical tungsten electrostatic probe positioned 6.5 cm below the magnet mid-plane. The main plasma generation region is assumed to correspond to the volume located directly beneath the ECR zones.

In the simulations, only a fraction of the total chamber volume is considered, corresponding to the primary plasma production region extending below the ECR sources. Both the neutral gas and ion temperatures are fixed at 600 K. The surface recombination probability of atomic hydrogen is set to $\gamma_r = 0.1$, a commonly adopted value for stainless-steel walls.

The model developed in this work was used to perform simulations under the same operating conditions adopted by Yang *et al.* [59]. The resulting electron densities and electron temperatures for the pressure scan are shown in Figure 3.7, together with the predictions of the reference model and the corresponding experimental measurements.

The qualitative trend of the electron density is consistent with that predicted by the reference model, although a difference in slope can be observed. This discrepancy can be attributed to differences in the collisional energy loss curve adopted by Yang *et al.* and that computed in the present work (Figure 3.4). Indeed, simulations performed using the collisional energy loss data reported by Yang *et al.* yielded electron density profiles that were nearly coincident with those of the reference model. This result indicates that the model is particularly sensitive to the collisional energy loss curve.

From a quantitative perspective, both the original and the developed models significantly overestimate the experimental electron density. However, this discrepancy had already

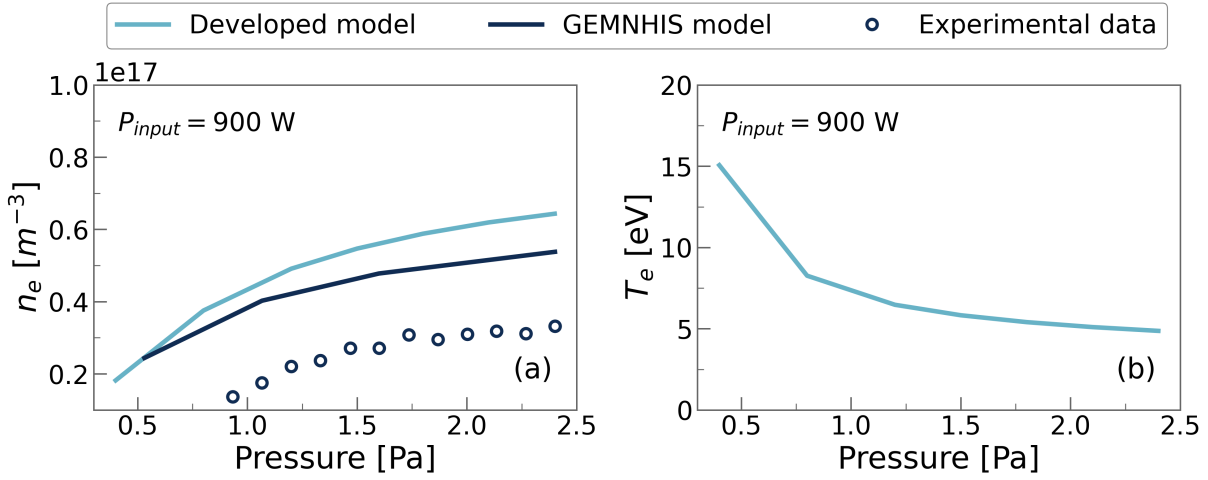


Figure 3.7: Comparison between the developed model, the GEMNHIS model of Yang *et al.* [59], and the experimental measurements reported in their work for the ECR discharge. (a) Electron density and (b) electron temperature as functions of gas pressure at constant input power, $P_{\text{input}} = 900 \text{ W}$.

been discussed in the original work and was attributed to an overestimation of the absorbed power. The modeled volume represents only a fraction of the total plasma volume and is located directly beneath the ECR source. It is therefore reasonable to assume that a portion of the total absorbed power is deposited outside the modeled region and does not contribute directly to sustaining the plasma within the simulated volume.

3.3.4. Discussion of results

The benchmark showed overall good agreement with the reference models. Nevertheless, some differences were observed, including with the model by Samuelli and Corr [47], which served as one of the primary references for the development of the present model. These discrepancies may arise from several factors. One important difference is the adopted reaction set and the associated cross-section data. Whenever available, the most up-to-date datasets were employed in the present work. Among the consequences of using different cross-section datasets is a variation in the collisional energy loss per electron-ion pair. As discussed in Subsection 3.3.3, the model is particularly sensitive to this quantity, which can lead to variations in the predicted trends.

Beyond the benchmarking results, the performed simulations provide additional insight into both the plasma dynamics and the behavior of the model itself. To illustrate these aspects, only the GEC Reference Cell is discussed here, although similar considerations can be drawn for the other systems as well.

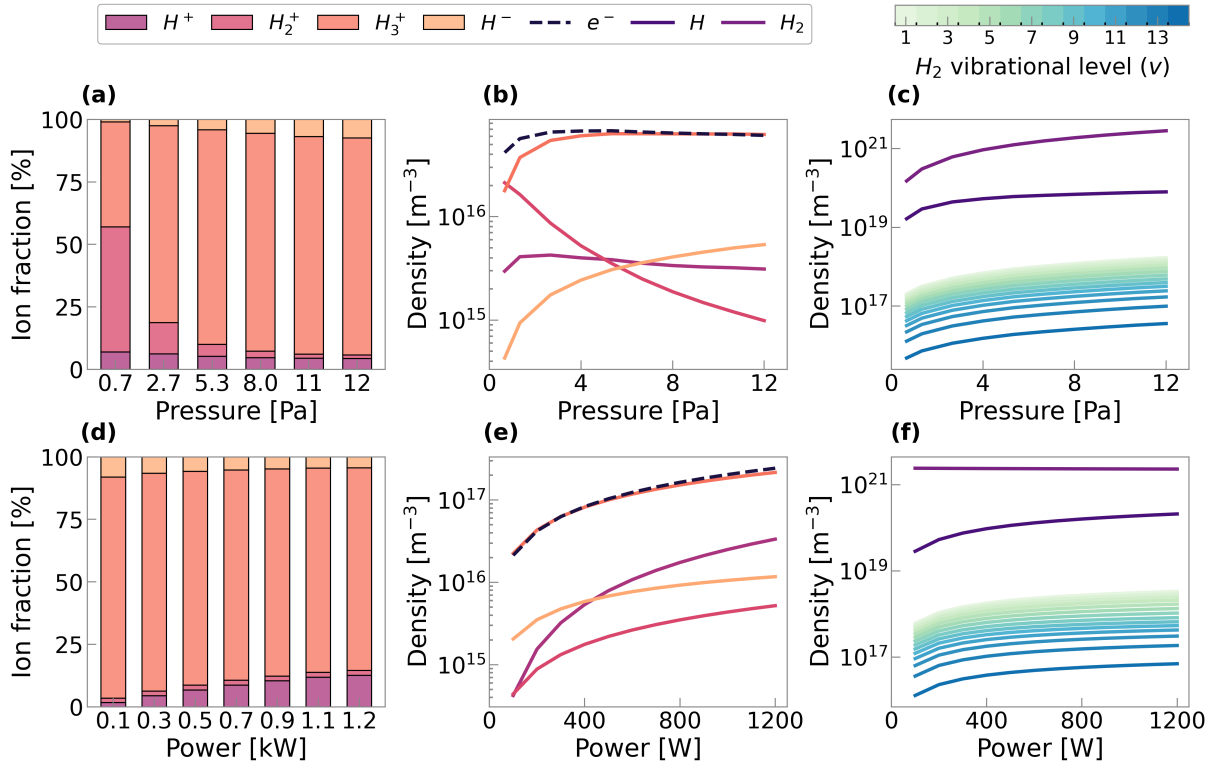


Figure 3.8: Plasma composition in the GEC Reference Cell as a function of pressure and input power. Pressure scan at constant $P_{\text{input}} = 300$ W: (a) ion fractions, (b) ion densities, and (c) neutral species densities. Power scan at constant $p = 10$ Pa: (d) ion fractions, (e) ion densities, and (f) neutral species densities.

Figure 3.8 shows the evolution of the plasma composition along the pressure and power scans. The most significant variations in the ionic composition are observed in the pressure scan. In contrast, the power scan exhibits only a gradual and approximately linear increase in the H^+ fraction.

During the pressure scan the relative abundances of the different species vary substantially, with some species even exchanging their dominant roles along the scan. At the lowest pressure, the plasma consists of approximately 50% H_2^+ , 42% H_3^+ , 7% H^+ , and a small remaining fraction of H^- . As the pressure increases, the composition progressively shifts, reaching approximately 1.4% H_2^+ , 87% H_3^+ , 4.3% H^+ , and 7.5% H^- at the highest pressure considered.

Such a pronounced behavior is associated with a variation in the chemical equilibrium³, which is determined by the balance between the production and loss terms of each species.

³In this specific context, the expression *chemical equilibrium* is extended to refer to the full set of reactions (both chemical and physical processes) included in the model.

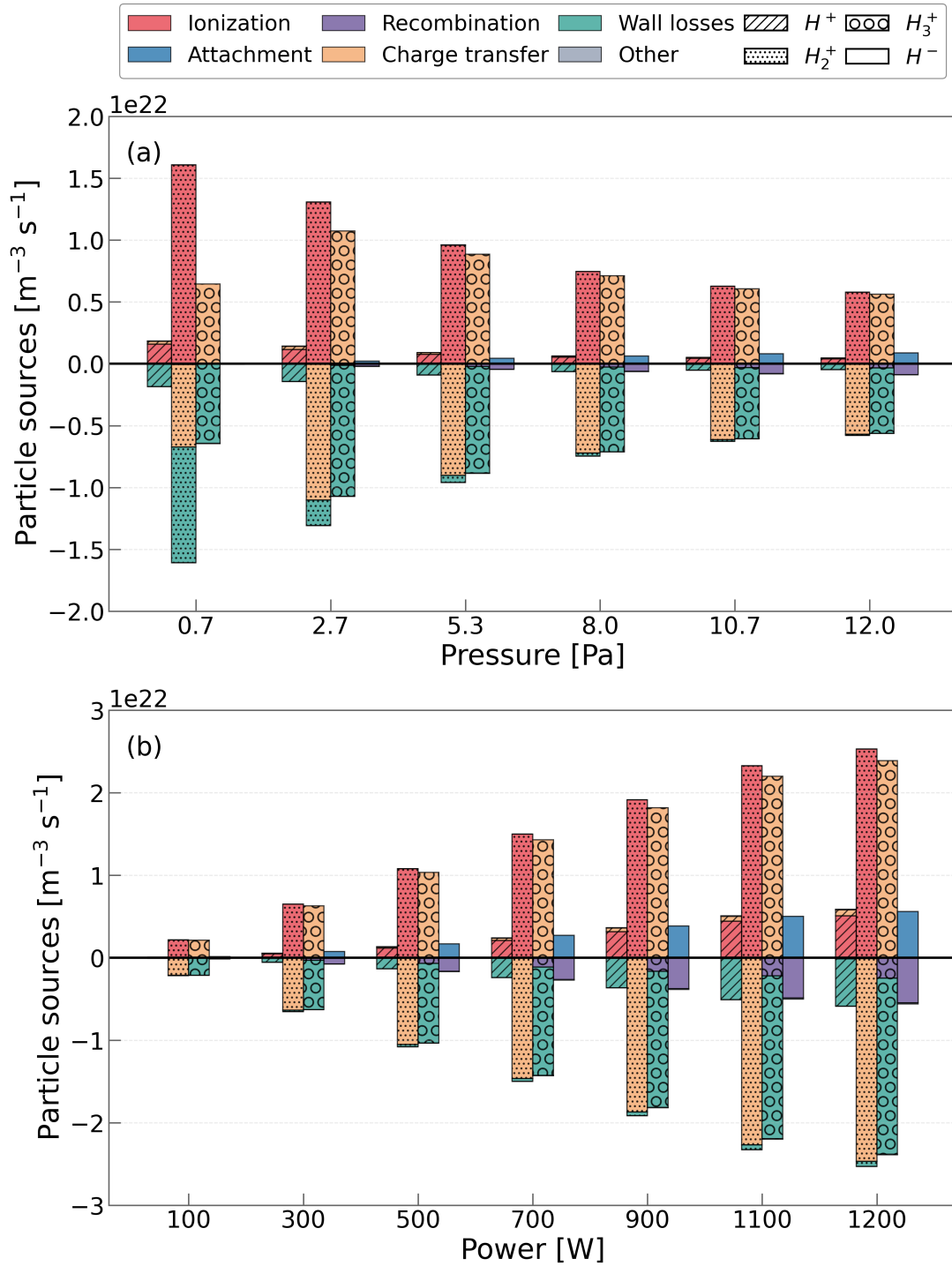


Figure 3.9: Contribution of the different physical processes to the source and loss rates of the charged species H^+ , H_2^+ , H_3^+ , and H^- in the GEC Reference Cell. Positive and negative values denote particle production and loss, respectively. (a) Pressure scan at constant $P_{\text{input}} = 300 \text{ W}$. (b) Power scan at constant $p = 10 \text{ Pa}$.

This interpretation is supported by Figure 3.9, which reports the contributions of the different physical processes to the source and loss rates of the charged particles. It can be observed that, during the power scan, all production and loss terms increase simultaneously, without significantly modifying their relative contributions. In contrast, along the pressure scan, the relative importance of the different processes changes substantially.

As the pressure increases, the ionization source terms decrease for all ion species, whereas the charge-exchange reaction responsible for the formation of H_3^+ is enhanced. The reaction can be written as



As a consequence, this process progressively depletes the H_2^+ population, leading to a reduction in its density and, therefore, in its wall-loss rate, which is directly proportional to the species density. At the same time, the increasing H_3^+ concentration results in higher wall losses for this ion. The growth of the H_3^+ population eventually slows down because the charge-exchange rate decreases as the H_2^+ density becomes progressively lower, reducing the availability of one of the reactants. For low-pressure plasmas, the observed increase in the H_3^+ concentration with pressure, driven by the enhancement of charge-exchange processes, is a well-established trend reported in the literature for both experimental and numerical studies [120, 121].

An additional interesting observation concerns the behavior of the electron temperature across all the power scans reported in this section. While the electron temperature varies significantly with pressure, it appears to be only weakly affected by changes in the input power. This behavior is physically reasonable, since the electron temperature governs the rate coefficients of many plasma reactions and therefore tends to adjust to values that sustain the overall chemical equilibrium. The latter has been observed to depend strongly on pressure, while showing a much weaker sensitivity to input power.

It can thus be inferred that, within the range of operating conditions considered, the electron temperature is primarily determined by the chemical equilibrium and is only weakly coupled to the input power. For a given chemical equilibrium, the total energy lost per electron is essentially fixed. Consequently, variations in the absorbed power are mainly accommodated through changes in the electron density rather than in the electron temperature.

It is also reasonable to conclude that changes in the input power have a limited impact on the chemical equilibrium itself because the plasma remains weakly ionized throughout the investigated parameter range. The densities of neutral species exceed those of charged particles by several orders of magnitude, effectively acting as an infinite reservoir. As

a result, ionization processes can significantly increase the charged particle population without appreciably modifying the concentrations of the neutral reactants.

4 | Case study of Deuterium plasma in the GyM Linear Plasma Device

The developed 0D model has been applied to the case study of deuterium plasma in GyM. A comparison with experimental data has been carried out with the dual purpose of validating the code for deuterium operation and investigating the plasma behavior and composition in the device.

Subsequently, GyM has been simulated using SOLPS-ITER in order to compare the predictions of the two codes and identify and understand possible discrepancies. In this context, the modeling assumptions adopted by SOLPS-ITER for molecular ions have also been investigated. This activity represents the in-depth study carried out as part of the *Honours Programme* in "Scientific Research in Industrial Engineering - Nuclear Science and Technology".

A brief description of the GyM device and the experimental setup is provided in Section 4.1, together with an overview of the experimental campaigns considered in this work. The simulation setups adopted for both SOLPS-ITER and the 0D model are described in Section 4.2. The comparison between the experimental measurements and the global model predictions is presented and discussed in Section 4.3. Finally, the comparison between the 0D model and SOLPS-ITER simulations is reported in Section 4.4.

4.1. Experimental setup

GyM is a linear plasma device operated at the Istituto per la Scienza e Tecnologia dei Plasmi of the Consiglio Nazionale delle Ricerche in Milan [122]. The facility was built in 2008 to investigate fundamental plasma physics phenomena, such as turbulence and coherent structures, which are characteristic of the tokamaks SOL. Since 2014, the GyM experimental program has mainly focused on plasma-material interaction (PMI) studies

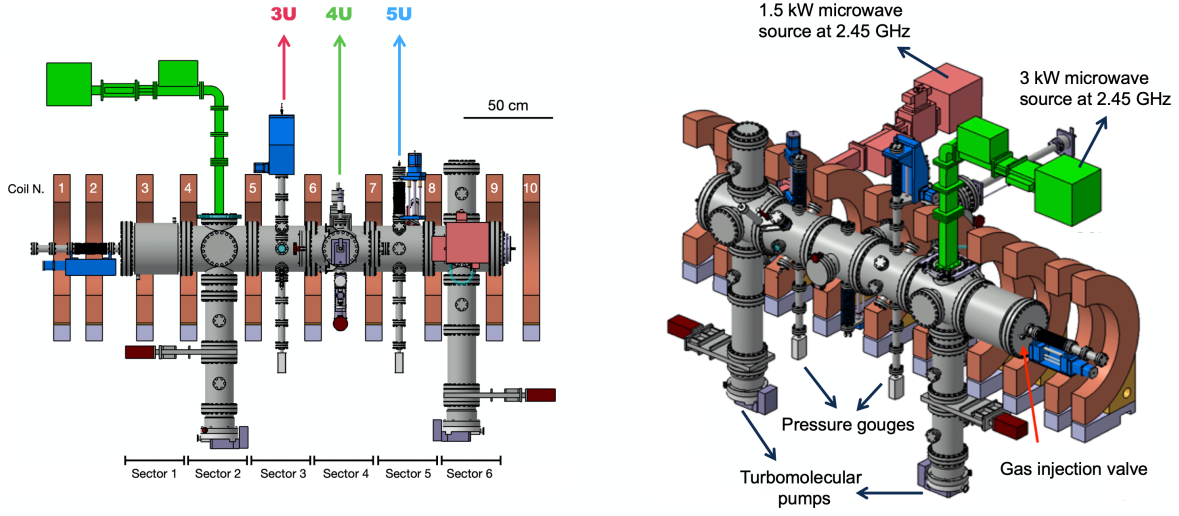


Figure 4.1: Rendering of the GyM linear plasma device, showing the locations of the ECRH sources, turbo-molecular pumps, gas injection valve, pressure gauges, and the three Langmuir probes (3U, 4U, and 5U) used for electron density and temperature measurements. Adapted from [36].

relevant to magnetic-confinement fusion devices [36].

GyM consists of a cylindrical vacuum chamber made of stainless steel (AISI 304L), with a radius of 0.125 m and a length of 2.11 m. It is equipped with two turbomolecular pumps, a gas injection system, ten magnetic field coils, and two 2.45 GHz magnetron sources providing a total maximum microwave power of 4.5 kW. A comprehensive set of diagnostics is installed on the machine, including two pressure gauges and three Langmuir probes. The vessel is conventionally divided into six sectors, and the probes, referred to as 3U, 4U, and 5U, are located in the corresponding sectors. In addition, two manipulator systems are available for PMI experiments [36]. A rendering of the device, showing the main components, is reported in Figure 4.1.

Each magnetic coil is an oxygen-free copper coil surrounding the vacuum vessel. They are connected in series generating an axial magnetic field configuration, which can be adjusted by varying the current flowing through the solenoid (I_{coils}), in the range 560-640 A, depending on the specific objectives of the experiment [36].

The plasma is sustained by *Electron Cyclotron Resonance Heating* (ECRH), an electron heating mechanism that exploits the resonance between the microwave frequency generated by the magnetrons and the electron cyclotron frequency Ω_e . As discussed in Subsection 1.2.1, Ω_e depends on the magnetic field strength. Consequently, resonance

Table 4.1: Summary of the main operational and plasma parameters of GyM [36].

Parameter	Value
Sources	2 Magnetrons at 2.45 GHz, Power of 1.5 kW and 3 kW, Steady-state
B field	≤ 0.13 T
Base pressure	$5.0 \cdot 10^{-6}$ Pa
Working pressure	$1.0 \cdot 10^{-3}$ – $1.0 \cdot 10^{-1}$ Pa
Electron density n_e	$\leq 1.0 \cdot 10^{17}$ m $^{-3}$
Electron temperature T_e	≤ 15.0 eV
Ion temperature T_i	≤ 0.1 eV
Ion flux Γ	$\leq 1.0 \cdot 10^{21}$ ions $\cdot$ m $^{-2}$ s $^{-1}$
Ion fluence Φ	$1.0 \cdot 10^{25}$ ions $\cdot$ m $^{-2}$ (After 7 h experiment)
Plasma diameter	0.25 m

occurs only within a limited spatial region, known as the *resonance layer*, defined by the locus of points where $B = 87.5$ mT. For the magnetic configurations typically employed in GyM, the resonance layer is located in sector 2U, which therefore acts as the primary plasma source region [36].

The main operational conditions and plasma parameters of GyM are summarized in Table 4.1.

In this work, two experimental campaigns were selected for comparison with the global model predictions. The first campaign, conducted on 25/02/2025, was carried out at a constant inlet gas flow rate of $\Gamma_{\text{feed}} = 13$ sccm, while the input power was varied between 320 and 1600 W. The second campaign, performed on 26/02/2025, was carried out at a constant input power of $P_{\text{input}} = 1300$ W, while the inlet gas flow rate was varied from 5 to 30 sccm. In both campaigns, the coil current was kept constant at $I_{\text{coil}} = 600$ A.

The neutral pressure was measured using a capacitive pressure gauge, whereas the electron density and electron temperature were obtained from Langmuir probe measurements. Conversely, the fraction of absorbed power relative to the injected microwave power, $\eta = P_{\text{abs}}/P_{\text{input}}$, cannot be reliably determined experimentally and therefore must be treated as a model free parameter.

For comparison with the global model, the values measured by the Langmuir probes at the three axial locations (3U, 4U, and 5U) and at different radial coordinates were volume-averaged over the region between 3U and 5U. This was achieved by integrating the measured quantities assuming a linear interpolation between adjacent axial positions and subsequently dividing by the corresponding total volume.

4.2. Simulation setup

In this section, the simulation setups and modeling assumptions are described. The definition of the SOLPS-ITER simulations is presented in Subsection 4.2.1. The 0D model is discussed afterwards in Subsection 4.2.2, where the setups used both for the comparison with experimental measurements and with SOLPS-ITER are described.

4.2.1. SOLPS-ITER

All the SOLPS-ITER simulations presented in this work were performed using version 3.0.10 of the code. The setup begins with the definition of the geometry and computational mesh. Since the code was originally developed for tokamaks and only later extended to LPDs, some peculiarities arise in the treatment of these geometries. In this case, the problem is reduced to a two-dimensional domain by exploiting the cylindrical symmetry around the device axis rather than the toroidal symmetry typical of tokamaks. Consequently, the simulation domain consists of half of the device cross-section, with the x- and y-directions corresponding to the axial and radial coordinates, respectively. Azimuthal (z) transport is not explicitly treated.

The construction of the computational mesh for linear machines starts from the reconstruction of magnetic equilibria for a coil current $I_{coil} = 600A$, following the procedure developed in [123]. The B2.5 quadrilateral mesh is composed of 75 cells in the axial (x) direction and 15 cells in the radial (y) direction. The EIRENE triangular mesh is then generated on top of it using the Tria and Triageom utilities. The resulting computational grid, obtained by superimposing the two meshes, is shown in Figure 4.2.

The boundary conditions are specified in the `b2.boundary.parameters` input file, following choices that have been well validated in the literature [89, 91, 124]. At the two targets, corresponding to the two bases of the cylinder, sheath boundary conditions are applied. On the southern boundary, which coincides with the symmetry axis, zero particle and energy fluxes are imposed, together with a zero parallel velocity gradient for the momentum equation and a zero-current condition for the potential equation. Finally, on the northern boundary, which coincide with the vessel wall, an exponential decay length ($\lambda_n = 5 \text{ cm}$) is prescribed for both the density and energy equations, while the parallel velocity gradient and the current are again set to zero. Physical and chemical sputtering are deactivated.

The pumping effect is modeled in EIRENE by assigning a pumping speed (in L/s) to the

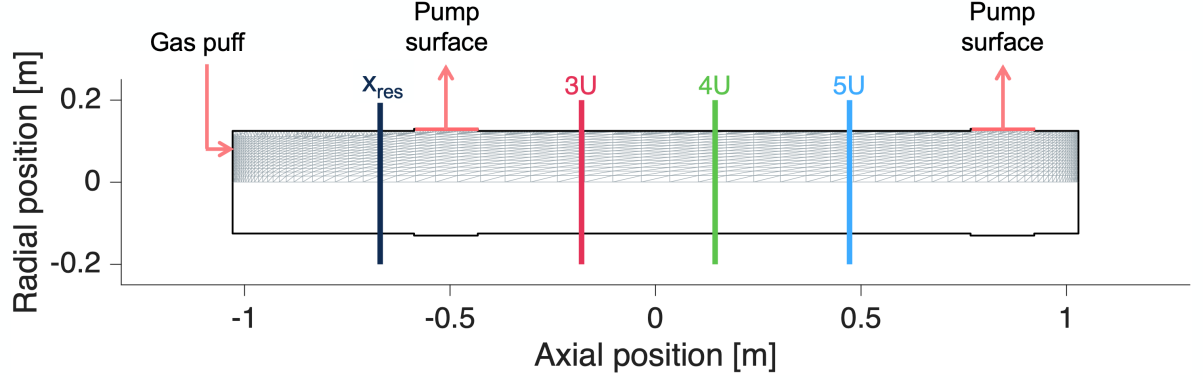


Figure 4.2: SOLPS-ITER computational domain adopted for the GyM simulations, showing the B2.5 (rectangular) mesh superimposed on the EIRENE (triangular) mesh, together with the vacuum vessel geometry, the locations of the pumping and gas injection systems, the positions of the Langmuir probes (3U, 4U and 5U), and the resonance position x_{res} for $I_{\text{coil}} = 600$ A.

pumping surface, given by [89]

$$S = A_{\text{pump}} \cdot p_a \cdot 3.638 \cdot \sqrt{\frac{T_{\text{wall}}}{m_{D_2}}} \quad (4.1)$$

where T_{wall} is the wall temperature in K, m_{D_2} is the molecular deuterium mass in amu, p_a is the absorption probability, and A_{pump} in cm^2 is the pumping surface area. Since SOLPS-ITER assumes cylindrical symmetry, the modeled pumping surface does not coincide with the actual pump geometry. Instead, it is obtained by revolving the pump cross-section around the device axis, yielding

$$A_{\text{pump}} = 2r \cdot 2\pi R \quad (4.2)$$

where R is the GyM radius and r is the pump radius.

The gas puff is specified in the `b2.neutrals.parameters` input file by prescribing a pure D_2 gas flow rate, expressed in s^{-1} , at the gas injection location shown in Figure 4.2.

To reproduce the ECRH effect, a volumetric power source must be defined. SOLPS-ITER allows the inclusion of external particle, momentum, and energy sources, with arbitrary radial and axial profiles specified through the `b2.sources.profile` input file. In this work, the ECRH source is implemented assuming a Gaussian power density absorption profile for electron only, centered at the axial resonance position, $x_{\text{res}} \simeq -0.67$ cm, cor-

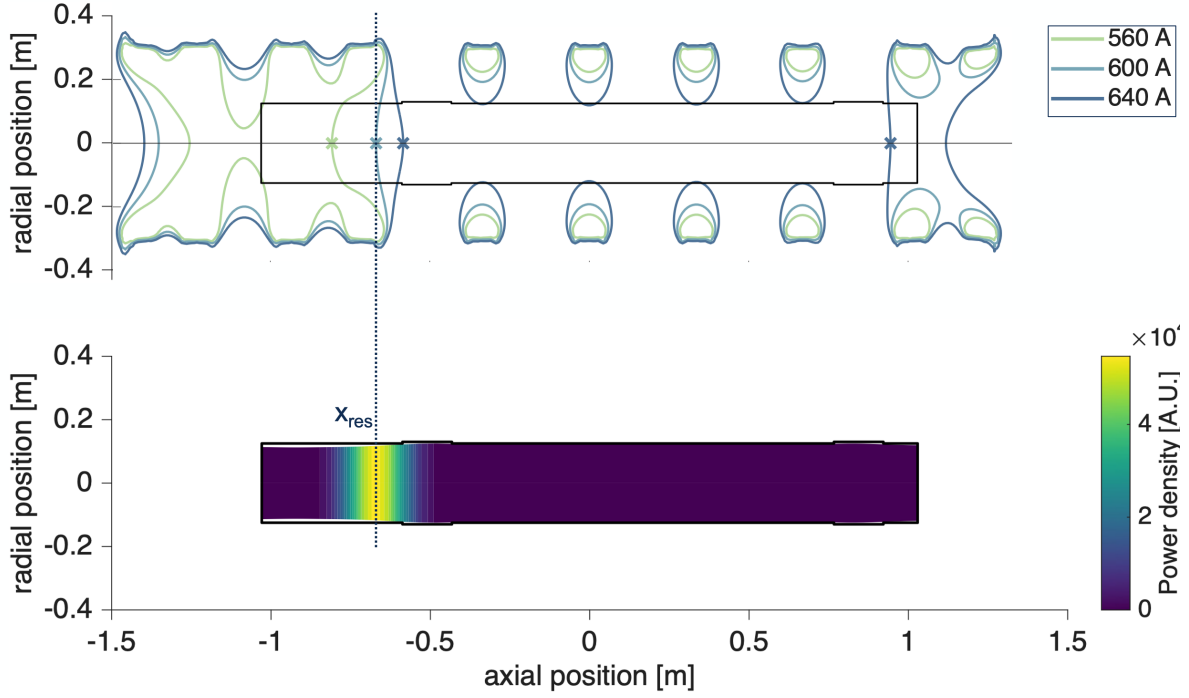


Figure 4.3: (a) Curves representing the loci of points satisfying the electron cyclotron resonance (ECR) condition, corresponding to $B = 87.6$ mT, for the three values of I_{coil} considered. (b) Contour plot of the volumetric power density source implemented in SOLPS-ITER to represent ECRH power deposition in the plasma.

responding to $I_{coil} = 600$ A. The total absorbed power is then obtained as the volume integral of the power density:

$$P_{abs} = \int \rho_{max} \exp \left\{ -\frac{(x - x_{res})^2}{\sigma^2} \right\} dV \quad (4.3)$$

where ρ_{max} is the peak power density and $\sigma = 0.1$ m.

The resulting profile is shown in Figure 4.3. The implemented power deposition model is deliberately simplified, featuring a power density that is uniform in the radial direction. A more realistic representation of the experimental density and temperature profiles would require a radially non-uniform deposition, with properly defined peaks. However, the primary objective of the present SOLPS-ITER simulations is the comparison with the 0D model. In this context, the simplified deposition profile does not represent a limitation; on the contrary, a more uniform power absorption facilitates a direct comparison between the two approaches.

Finally, the transport properties are defined through the `b2.transport.parameters` file,

where the value of the anomalous cross-field particle transport coefficient, $D_{\perp}$, is specified.

The values of p_a , P_{abs} , and $D_{\perp}$ are not directly available from experimental measurements and therefore must be calibrated to reproduce a selected experimental case. In this work, these parameters were taken from simulations performed by A. Villa [93], reproducing an experimental configuration with $I_{coil} = 600$ A, $P_{input} = 1300$ W, and $\Gamma_{feed} = 13$ sccm, yielding optimized values of $p_a = 0.0075$, $P_{abs} = 408$ W, and $D_{\perp} = 0.75$ m²/s. This reference case was reproduced in this work using the simplified power deposition profile described above.

Starting from this reference simulation, two parameter scans were performed. In the first scan, the gas feed rate was fixed at $\Gamma_{feed} = 13$ sccm while the absorbed power P_{abs} was varied from 200 to 408 W. In the second scan, the absorbed power was fixed at $P_{abs} = 408$ W while Γ_{feed} was varied from 5 to 25 sccm. These simulations do not correspond to specific experimental discharges but rather explore representative operating conditions within the GyM parameter range. In fact, their purpose is not experimental validation, but rather the comparison between the SOLPS-ITER simulations and the 0D model.

To enable a direct comparison between the 2D and 0D results, volume-averaged quantities were evaluated. The electron temperature and particle densities were integrated over the computational domain in the radial and axial directions under the assumption of cylindrical symmetry, and subsequently normalized by the total volume.

4.2.2. 0D model

The developed global model has been used both for comparison with GyM experimental data and with SOLPS-ITER simulations. Different setups were adopted for the two applications.

In both cases, the device geometry was represented as a cylinder, with diffusion boundary conditions imposed on the lateral wall to account for the presence of magnetic confinement. The gas and ion temperatures were assumed to be equal and were kept constant at a value determined as described in Section 4.3. The recombination probability was set to $\gamma_r = 0.1$, a typical value for stainless steel surfaces [59], while the quenching probability was fixed at $\gamma_Q = 1$.

For the simulations aimed at comparison with experimental data, the values of $D_{\perp}$ and η are treated as free input parameters and have therefore been optimized through dedicated parameter scans. The gas pressure associated with each experimental configuration,

which constitutes an input parameter for the global model, is measured by means of a capacitive pressure gauge. Inlet gas flow rate and gas pressure are strictly related quantities; consequently, the experimental inlet gas flow rate scan is hereafter treated as a pressure scan.

For the comparison with SOLPS-ITER, the 0D simulations employ the same input parameters as the corresponding SOLPS-ITER simulations, ensuring consistency between the two approaches. Consequently, regardless of the value of $D_{\perp}$ optimized against the experimental data within the 0D model, a fixed value of $0.75 \text{ m}^2/\text{s}$ is assumed. Furthermore, since the SOLPS-ITER scan does not correspond to experimental cases, the parameter η is not involved and the absorbed power, P_{abs} , is directly prescribed. Finally, the pressure cannot be obtained from experimental measurements in this case and is therefore evaluated from the balance between the injected and pumped particle fluxes. The latter is calculated according to the SOLPS-ITER pumping model described in Subsection 4.2.1 and Equation 4.1. The resulting pressure, in Pa, is given by:

$$p = \frac{\Gamma_{feed} k_B T_g}{2A_{pump} \cdot p_a \cdot 3.638 \cdot 10^{-3}} \sqrt{\frac{m_{D_2}}{T_g}} \quad (4.4)$$

where Γ_{feed} is expressed in s^{-1} and k_B is the Boltzmann constant.

To gain a deeper understanding of the implications of the SOLPS-ITER assumptions regarding molecular ions, a *frozen mode* switch was implemented in the global model to reproduce the same conditions. When activated, this mode excludes the user-selected *frozen species* from the charge balance equation, wall interactions and losses, and pumping processes. Simulations were then performed both with and without the frozen conditions enabled. In frozen mode D_2^+ and D_3^+ were defined as frozen species, while D^- was not included at all, consistently with the SOLPS-ITER treatment.

4.3. Global model validation and analysis of GyM

The GyM simulations with the global model first required the evaluation and optimization of the free parameters.

The first step consisted in defining the gas temperature. In GyM, this quantity is not directly measured and is typically assumed to be 300 K, with an ion temperature $T_i \leq 0.1 \text{ eV}$. In this work, the effect of varying the gas temperature was investigated by performing a set of simulations at fixed $D_{\perp}$ and η , while progressively increasing T_g starting from 300 K. It was observed that increasing T_g improves the agreement of the

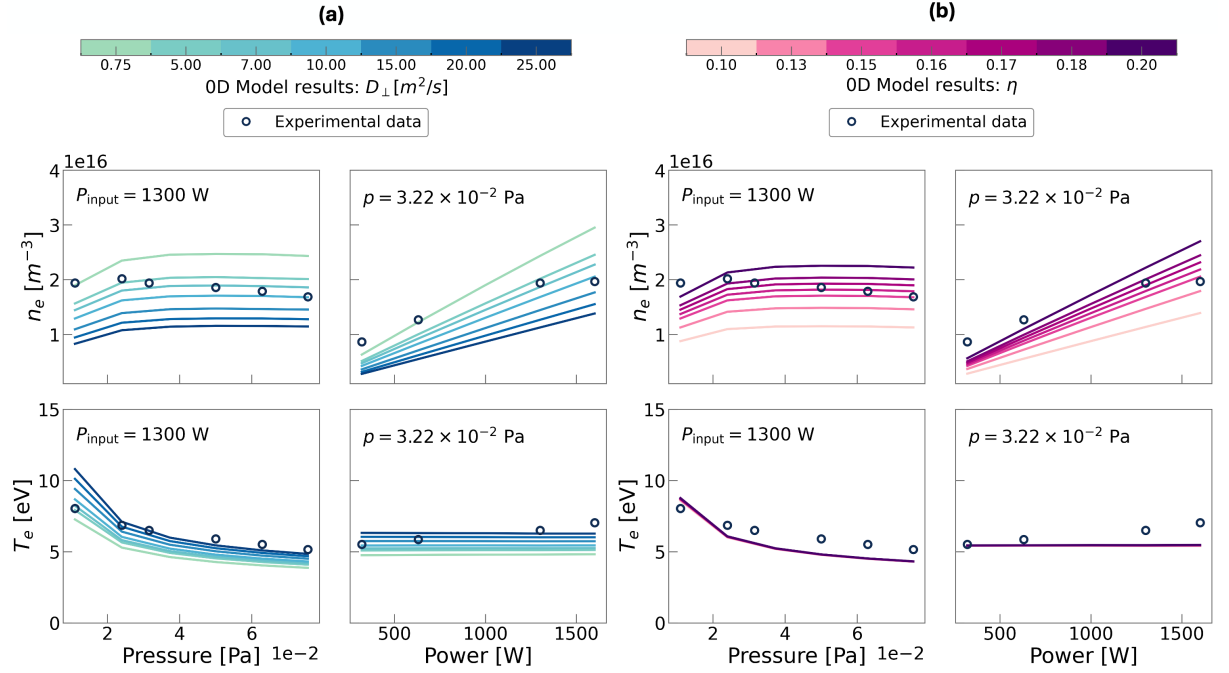


Figure 4.4: Optimization scans of the anomalous transport coefficient $D_{\perp}$ and the power absorption fraction η , compared with GyM experimental values. (a) Scan of $D_{\perp}$ at fixed $\eta = 0.15$. (b) Scan of η at fixed $D_{\perp} = 10 \text{ m}^2/\text{s}$.

electron temperature profile with the experimental data; however, the slope of the electron density profile varies with T_g in a way that deviates in the opposite direction with respect to the measurements. This suggests that no significant gas heating is likely to occur in the system. This conclusion is further supported by the fact that electron elastic energy losses account for an almost negligible fraction of the total dissipated power, thus not justifying a substantial increase in gas temperature. For these reasons, T_g was limited to 350 K, which is the value assumed in all simulations reported below.

For the evaluation of $D_{\perp}$ and η , dedicated parametric scans were performed by varying one quantity at a time while keeping the other fixed. The optimal values were identified by minimizing the *Normalized Root Mean Square Error* (NRMSE) with respect to the experimental measurements. An example of the optimization procedure for each parameter is shown in Figure 4.4. It is worth noting that the electron temperature curves are essentially unaffected by variations in η , consistently with the decoupling between electron temperature and absorbed power already discussed in Subsection 3.3.4. In contrast, variations in $D_{\perp}$ directly affect plasma wall losses, thereby modifying the chemical equilibrium. As a consequence, increasing $D_{\perp}$ shifts the electron temperature curves upward while reducing the electron density.

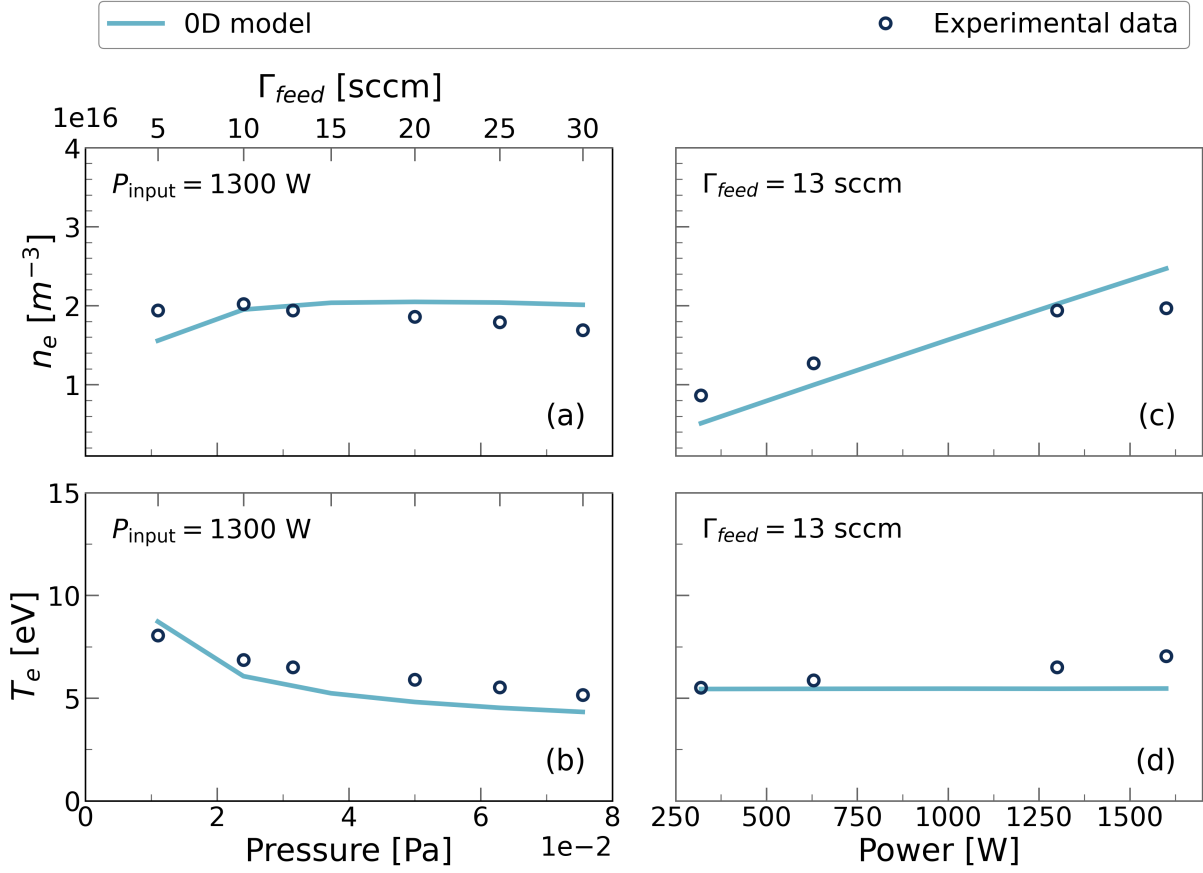


Figure 4.5: Comparison between global model results and experimental measurements on GyM, using optimized parameters $D_{\perp} = 10$ m²/s and $\eta = 0.18$. (a) Electron density and (b) electron temperature as functions of gas pressure at constant input power, $P_{input} = 1300$ W; (c) electron density and (d) electron temperature as functions of input power at fixed inlet gas flow rate, $\Gamma_{feed} = 13$ sccm.

A range of optimal parameter combinations was identified, spanning from $D_{\perp} = 5$ m²/s and $\eta = 0.15$, which provides the best agreement with the experimental electron density measurements (NRMSE = 19.3%), to $D_{\perp} = 20$ m²/s and $\eta = 0.23$, which yields the best agreement for the electron temperature (NRMSE = 20.3%). The purpose of a global model is not to achieve an exact reproduction of a specific experimental configuration, but rather to provide reliable estimates of the plasma parameters and to capture their qualitative trends under variations of the input conditions. Therefore, identifying a unique optimum set of free parameters is beyond the scope of this work. In the following, an intermediate parameter set, with $D_{\perp} = 10$ m²/s and $\eta = 0.18$, is adopted as the reference case. The corresponding simulation results are presented in Figure 4.5. Overall, the model reproduces the experimental trends well, regardless of the optimized absolute values, confirming its predictive capability.

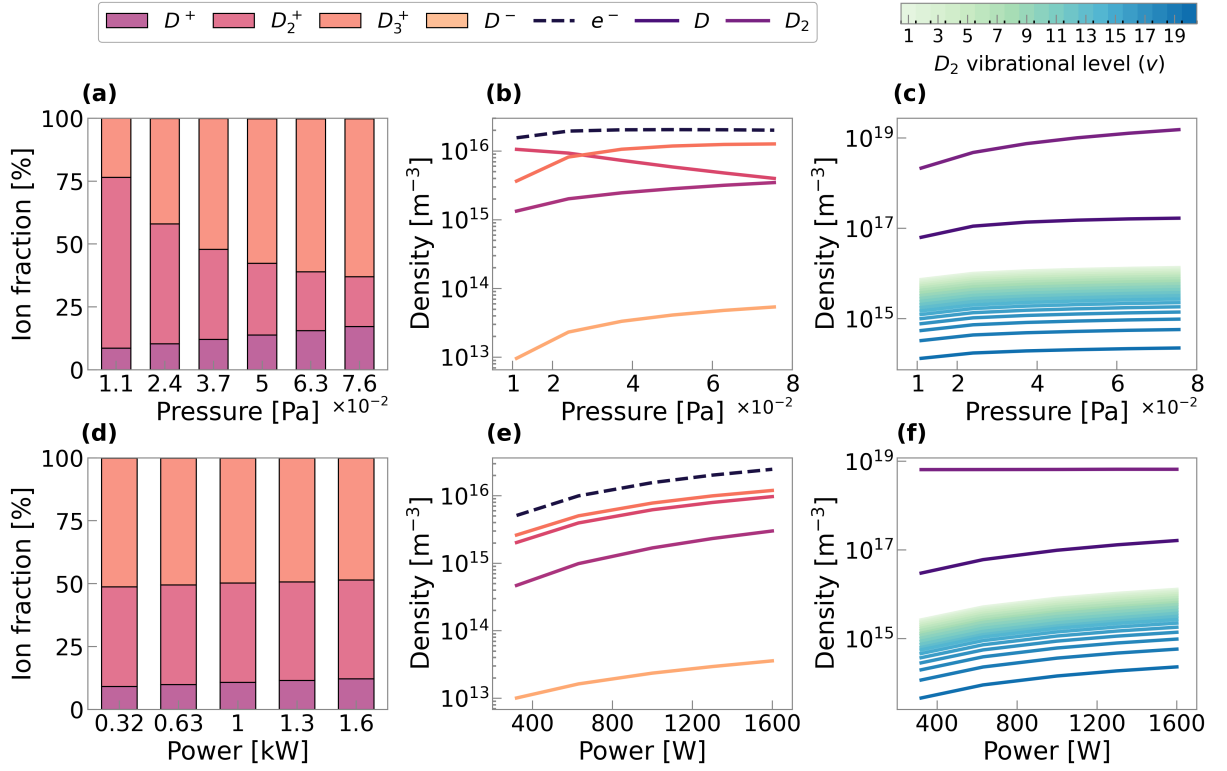


Figure 4.6: Plasma composition in GyM as a function of pressure and input power, using optimized parameters $D_{\perp} = 10 \text{ m}^2/\text{s}$ and $\eta = 0.18$. Pressure scan at constant $P_{\text{input}} = 1300 \text{ W}$: (a) ion fractions, (b) ion densities, and (c) neutral species densities. Power scan at constant $\Gamma_{\text{feed}} = 13 \text{ sccm}$: (d) ion fractions, (e) ion densities, and (f) neutral species densities.

The estimated $D_{\perp}$ may appear relatively large when compared with the value used in the SOLPS-ITER simulations, $D_{\perp} = 0.75 \text{ m}^2/\text{s}$. However, it is important to consider the different role played by this parameter in the two codes. In SOLPS-ITER, which is a 2D fluid code, particle transport is explicitly modeled and spatially resolved. In contrast, a 0D global model does not account for spatial effects, and the diffusion coefficient acts primarily as an effective parameter describing particle losses to the lateral walls. Consequently, in the present model, $D_{\perp}$ should be interpreted as an estimate of the effective diffusion coefficient at the plasma boundary rather than in the inner region.

In the SOLPS-ITER simulations performed in this work, a radially uniform diffusion coefficient was assumed. However, studies available in the literature for other kinds of plasmas in GyM utilize more sophisticated radial transport profiles. For instance, Mombelli *et al.* [124] observed that a radially increasing profile $D_{\perp} \propto r^2$ - scaling from $1 \text{ m}^2/\text{s}$ in the inner region to $10 \text{ m}^2/\text{s}$ near the walls - achieves better agreement with experimental

data. Therefore, the values obtained from the optimization of the global model remain physically plausible despite being significantly larger than the uniform coefficient adopted in the reference SOLPS-ITER simulations.

From the global model simulations, the plasma composition can be estimated. Figure 4.6 shows the results obtained for the optimized reference case. In all the simulated conditions, D^+ is predicted to be the minor positive ion species. Instead, molecular ions dominate the plasma composition, with the fraction of D_2^+ decreasing from 68% to 20% and that of D_3^+ increasing from 23% to 63% as the pressure increases. As a result, these two molecular ions together account for more than 80% of the positive ion population over the entire pressure range considered.

The negative ion D^- fraction is essentially negligible in this case, with a density approximately two orders of magnitude lower than that of the positive ion species. In contrast, for the hydrogen case discussed in Subsection 3.3.4, D^- represented a minor but non-negligible plasma component. This difference is mainly attributed to the lower dissociative attachment cross sections associated with vibrationally excited D_2 molecules compared to hydrogen, as reported in the literature reviewed in Subsection 2.3.5 [75].

The plasma composition is not directly measured in GyM, yet it is a key quantity for several applications, including plasma-surface interaction and erosion studies. In this context, the developed 0D model can play an important role, as it is able to describe complex plasma chemistry with a level of detail that is often not achievable in higher-dimensional simulations.

4.4. Comparative analysis of SOLPS-ITER and the 0D model

The SOLPS-ITER modelling activity was initiated by simulating the reference experimental case at $P_{input} = 1300$ W and $\Gamma_{feed} = 13$ sccm. The corresponding results are compared with the experimental measurements in Figure 4.7.

It can be observed that the simulation is unable to reproduce the radial shape of the electron density and temperature profiles. This discrepancy is mainly attributed to the simplified power absorption profile adopted. In fact, it is assumed to be radially uniform, whereas experimental observations reveal the presence of localized radial spikes. Reproducing such features would require a more realistic power deposition profile including appropriately positioned radial peaks.

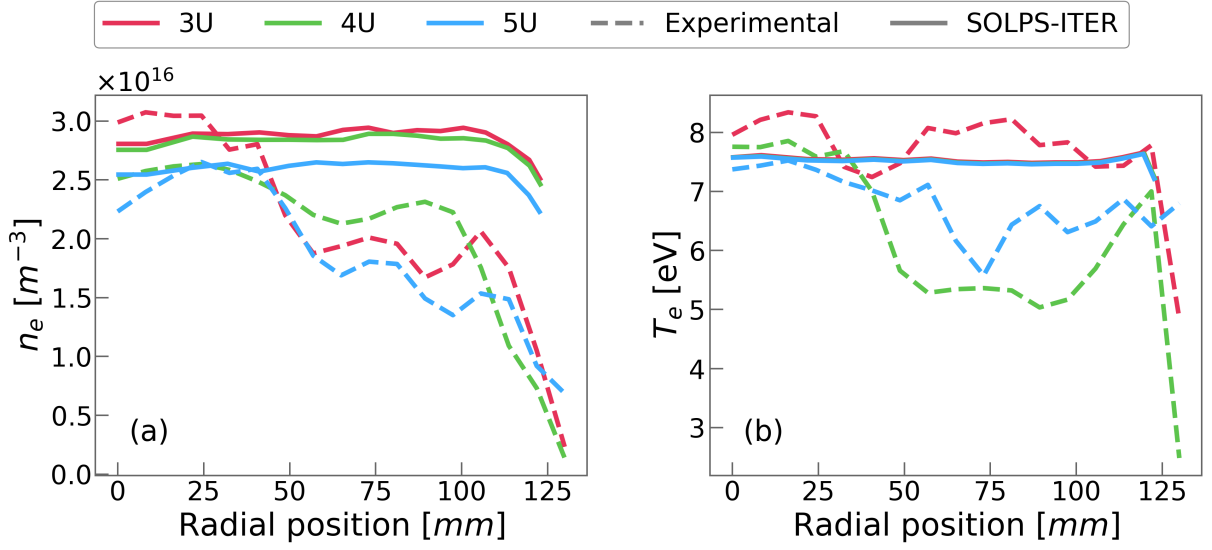


Figure 4.7: Comparison between SOLPS-ITER predictions and experimental measurements of the radial profiles of (a) electron density and (b) electron temperature at the 3U, 4U, and 5U axial positions for the reference operating condition ($P_{input} = 1300$ W, $\Gamma_{feed} = 13$ sccm).

Nevertheless, for the purposes of the present work, a more homogeneous power absorption profile facilitates the comparison between SOLPS-ITER and the 0D model. Consequently, the primary objective is not to reproduce the exact radial profile shape, but rather to achieve agreement in the order of magnitude of the plasma parameters. This condition is satisfied by the simulations in the central region of the device, where GyM exhibits a higher degree of radial uniformity in both electron density and temperature. This region is also employed for PWI sample exposure studies. Indeed, the samples have a maximum radial extension of approximately 2 cm, ensuring that they experience nearly identical plasma conditions over their entire surface. Therefore, when focusing on PMI studies, the most relevant plasma parameters to be reproduced in the GyM simulations are those characterizing this central region.

The results of the comparison between SOLPS-ITER and the 0D simulations are reported in Figure 4.8. The 0D model under standard conditions (i.e., without activating the frozen mode) yields approximately twice the electron density and lower electron temperatures with respect to SOLPS-ITER. When the frozen condition is activated in the global model, the predicted electron densities become almost coincident with those obtained from SOLPS-ITER, and the electron temperature also shows improved agreement. This suggests that the discrepancy between the global model and SOLPS-ITER does not arise from limitations of the 0D modeling approach, but rather from the assumptions

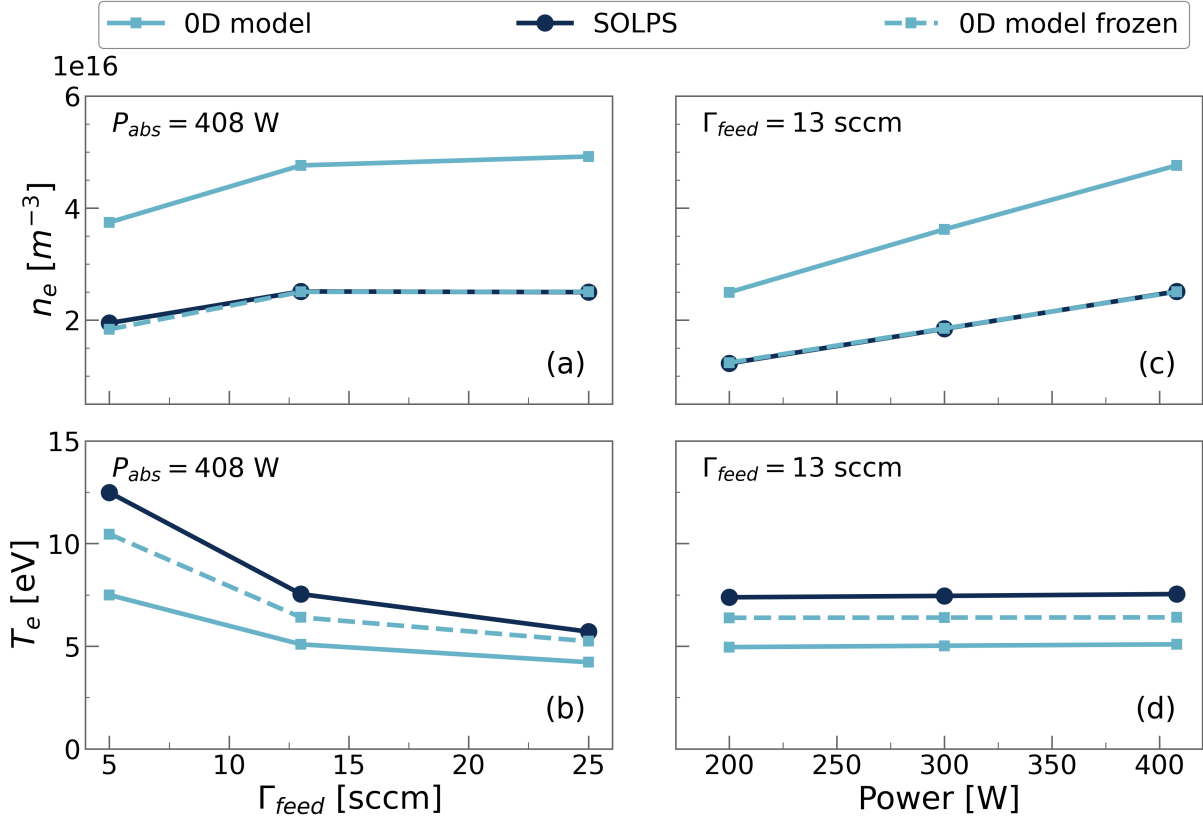


Figure 4.8: Comparison of the 0D model (without frozen condition), the 0D model with the frozen condition, and the SOLPS-ITER results for GyM. (a) Electron density and (b) electron temperature as functions of the inlet gas flow rate at constant input power, $P_{abs} = 408$ W; (c) electron density and (d) electron temperature as functions of input power at inlet gas flow rate, $\Gamma = 13$ sccm.

implemented in SOLPS-ITER.

To assess the main implications of these assumptions on the modeled plasma dynamics, further analyses have been conducted. However, a preliminary observation can already be made. In Subsection 4.3, the GyM plasma composition has been estimated using the global model, showing that the plasma is predominantly composed of molecular ions. This already suggests that, in the considered conditions, these species are not short-lived, as assumed for the validity of the static approximation. This finding therefore raises questions regarding the SOLPS-ITER modeling approach, in which molecular ions are neither included as fluid species nor transported within EIRENE.

The left panel of Figure 4.9 shows a bar plot of the ion plasma composition, where all densities are normalized to the electron density. The results obtained from SOLPS-ITER are compared with those of the 0D model. In a quasi-neutral plasma composed only of

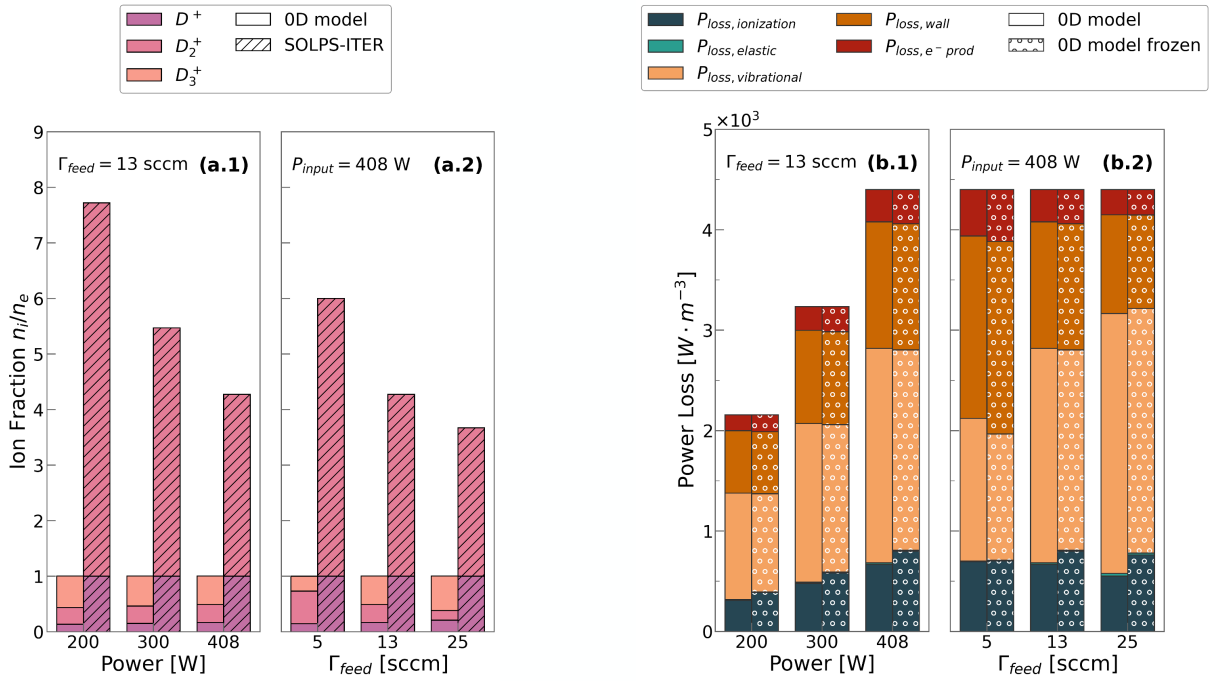


Figure 4.9: On the left: ion plasma composition normalized to the electron density, comparing SOLPS-ITER results with the 0D model. On the right: decomposition of power losses into all included channels, comparing the standard 0D model with the frozen-mode 0D formulation.

singly charged positive ions, the sum of ion densities should equal the electron density n_e (neglecting, for simplicity, the D^- contribution, which is found to be negligible in this case). Therefore, when normalized to n_e , this sum should be equal to unity. This condition is satisfied by the global model results but not by SOLPS-ITER. In the latter case, the electron density is fully balanced by the D^+ density alone, while the D_2^+ density ranges from approximately 2.7 to 6.7 n_e over the considered operating conditions.

This behavior is unphysical and stems from the fact that, not being treated as a fluid species, D_2^+ is not included in the charge balance. As a result, SOLPS-ITER effectively describes a plasma consisting only of D^+ , which, according to the global model, is instead the minor positive ion species. Consequently, D_2^+ accumulates in EIRENE until the D^+ density adjusts to enforce quasi-neutrality.

For the discrepancy in the electron density, further insight can be obtained by comparing the 0D simulations performed with and without the frozen mode activated. Recalling the general considerations discussed in Subsection 3.3.4, the electron population adjusts to balance the externally absorbed power according to the energy loss associated with each electron under the given operating conditions. Consequently, the observed variation in

electron density can be attributed to a variation in the energy loss per electron.

At constant absorbed power, such a variation may arise from a change in the plasma chemistry, leading to a different distribution of power loss channels. For constant pressure, instead, it may be given by a variation of the total absorbed power. Since the absorbed power is the same in the corresponding frozen and non-frozen simulations, the latter mechanism cannot explain the observed discrepancy. Moreover, the right panel of Figure 4.9 shows that the relative contributions of the different power loss channels remain nearly unchanged. Therefore, changes in the power loss distribution cannot account for the observed results either. Nevertheless, activating the frozen mode is found to increase the energy lost per electron by approximately 90-100%.

This can be explained by considering that, whenever an electron ionizes a D_2 molecule, the electron generated in the ionization process is effectively removed from the plasma. In fact, since the resulting D_2^+ ion is excluded from the charge balance, no net positive charge is created and, consequently, no additional electron can be retained in the plasma. As a result, ionization events contribute to power dissipation without increasing the electron population, effectively increasing the energy cost of electron-ion pair generation and leading to a lower equilibrium electron density.

This mechanism also explains another difference between the SOLPS-ITER and 0D simulations. Considering the reference experimental case, for the same input power, $P_{\text{input}} = 1300$ W, SOLPS-ITER predicts an absorbed power of $P_{\text{abs,SOLPS}} = 408$ W, whereas the global model yields $P_{\text{abs,0D}} \approx 230$ W. Thus, SOLPS-ITER requires nearly twice the absorbed power estimated by the global model to sustain the plasma. This is consistent with the finding that the effective energy loss per electron is approximately doubled under SOLPS-ITER-like modeling conditions.

5 | Conclusions and future developments

This thesis addressed the complexity of hydrogen and deuterium plasma modeling through the development, benchmarking, validation, and application of a global (0D) model, with particular focus on its use in the study of linear plasma devices (LPDs) for magnetic confinement fusion.

In this context, the present work pursued three main objectives: (i) the development and benchmarking of a global model for hydrogenic plasmas explicitly accounting for deuterium, (ii) the investigation of deuterium plasmas in the GyM LPD using this model, together with the validation of its predictions against experimental observations, and (iii) the assessment of the open issues related to the validity of the SOLPS-ITER modeling approach for molecular ions in LPDs.

The development of the global model is described in Chapter 3. It is intended for low-temperature ($\lesssim 20$ eV) and low-to-intermediate pressure ($\sim 10^{-2}$ - 15 Pa) plasmas sustained by electron heating. Owing to the general lack of dedicated deuterium modeling studies in the literature, it was first developed for pure hydrogen plasmas and subsequently extended to deuterium, with the reaction database constructed through physically justified assumptions whenever dedicated cross-section data were unavailable. It was benchmarked against two reference global models from the literature, by Samuelli and Corr [47] and by Yang *et al.* [59], across three plasma configurations, demonstrating predictive capabilities comparable to, and in some cases better than, those of the reference models.

Then in Chapter 4 the modeling activity performed on deuterium plasmas in GyM is described. In this context, both the 0D and SOLPS-ITER simulations were presented. The global model was applied to the selected experimental conditions. Two free parameters, the anomalous transport coefficient $D_{\perp}$ and the absorbed power fraction η , were optimized against the measurements. The final results reproduced the experimental trends in electron density and temperature, confirming its validity also for deuterium plasmas, and provided estimates of the plasma composition showing that molecular ions (D_2^+ and D_3^+)

dominate over the entire range of operating conditions considered.

Finally, a comparative analysis between SOLPS-ITER and the 0D model was performed to assess the validity of the modeling approach applied by SOLPS-ITER to molecular ions, whose validity in linear plasma devices is not guaranteed a priori. A frozen mode, reproducing the SOLPS-ITER molecular treatment, was implemented in the global model for this purpose. Under standard conditions, the 0D model showed significant discrepancies with SOLPS-ITER; activating the frozen mode, however, yielded almost perfect agreement, indicating that the mismatch originates from the SOLPS-ITER assumptions rather than from limitations of the 0D approach. Moreover, SOLPS-ITER predicted a plasma composed exclusively of D^+ , whereas the global model identified D^+ as the minor ion species, with D_2^+ – excluded from the charge balance in SOLPS-ITER – accumulating to densities exceeding the electron density by a large factor. These results suggest that the static approximation should not be applied to hydrogen molecular ions in a linear plasma device operating under GyM-like conditions.

All the three objectives outlined for this thesis were achieved. Beyond this, the work carried out allows some broader conclusions to be drawn regarding the role and reliability of the developed global model in the study of hydrogenic plasmas and in fusion relevant applications.

The benchmarking activity, carried out for three different hydrogenic plasma configurations, demonstrated that the model reliably reproduces the predictions of established references from the literature, and in several cases matches experimental data more closely. An analysis of the plasma composition and dynamics in terms of source and loss terms further confirmed the consistency of the model with the expected physical behavior, strengthening confidence in its underlying formulation.

The validation against GyM experimental data extended this assessment to deuterium plasmas. With only two free parameters tuned, $D_\perp$ and η , the model reproduced the measured trends in electron density and temperature over a representative range of input power and gas flow rate. This result also confirms the effectiveness of having explicitly adapted the model to deuterium – through a dedicated reaction database accounting for isotope-specific effects – rather than reusing a hydrogen model directly, as is common practice in the literature. A concrete example is the markedly lower D^- fraction predicted for deuterium compared to hydrogen, consistent with the lower dissociative attachment cross sections of vibrationally excited D_2 molecules reported in the literature, which a hydrogen-based treatment would not have captured.

Taken together, these results demonstrate that the developed 0D model is a reliable and

physically consistent tool for describing both hydrogen and deuterium plasmas within the investigated low-temperature, low-density regime, as validated against independent reference cases spanning two isotopically distinct systems.

This reliability is what makes the model useful for practical applications. It allows the interplay among different physical processes underlying the observed plasma behavior to be studied directly, as in the case of the decoupling between temperature and input power discussed in Subsection 3.3.4. It also gives access to quantities that are not directly measurable experimentally – most notably, in GyM, the full plasma composition. The model showed that the GyM deuterium plasma is dominated by molecular ions, D_2^+ and D_3^+ , rather than atomic ones, a result that experimental diagnostics alone could not have provided, and that has direct implications for plasma-surface interaction studies in the device.

The comparison with SOLPS-ITER adds a further dimension to these conclusions. Confronting the global model with a 2D fluid code made it possible to test its predictions against an independent and higher-fidelity approach, and, conversely, to use the global model to probe an assumption embedded in a code as established as SOLPS-ITER. This is, in itself, a confirmation of the role envisioned for global models in Section 2.3: their simplicity and direct link to the underlying physics make them well suited to expose hidden assumptions in higher-fidelity tools, which are often too complex to be interrogated directly.

The fact that activating the frozen mode in the 0D model reproduced the SOLPS-ITER results almost exactly, together with the unphysical D_2^+ densities predicted by SOLPS-ITER, provides strong evidence that the discrepancy originates specifically from molecular-ion modeling assumptions, rather than from some other unidentified difference between the two codes. This could not have been established by comparing SOLPS-ITER to experimental data alone, as any discrepancy could in principle have originated either from the molecular-ion modeling strategy or from other aspects of the model. This finding also implies that the short-lived assumption for molecular ions is not satisfied, and that the static approximation cannot be considered valid under these conditions. These results carry a practical consequence beyond GyM itself: they suggest that simulation results obtained with the current SOLPS-ITER treatment of molecular ions should be interpreted with caution whenever applied to plasma densities approaching or below those typical of linear plasma devices.

This work opens the way to several future developments, concerning both the model itself and its applications.

Regarding the development of the 0D model, several aspects could be further investigated and improved. The proposed deuterium reaction database could be further validated and improved through the identification of currently unavailable deuterium-specific data. In addition, the impact of adopting alternative modeling approaches for some of the most relevant reaction terms, such as wall processes, could be assessed. Furthermore, some of the assumptions currently adopted could be relaxed, such as the one of constant ion and neutral gas temperatures. Indeed, even under the operating conditions considered in this work, the presence of vibrationally excited molecules could lead to a non-negligible heating of the heavy species, an effect that deserves further investigation. This could be done by including dedicated power balance equations for ions and neutrals, allowing their temperatures to be determined self-consistently. Besides providing a more physically complete description, this extension would broaden the range of applicability of the model to hotter plasmas.

The model could also be exploited in several practical applications. Its predictive capability can support a variety of studies; for example, estimates of the plasma composition can be used to improve plasma-surface interaction and erosion analyses. Indeed, this application is already underway: predictions from the global model developed for GyM will provide composition-resolved ion fluxes as input to ERO2.0, a code for simulating plasma-wall interactions (PWI) and impurity transport in the plasma volume. This will replace the plasma composition currently predicted by SOLPS-ITER, which was shown to be inaccurate under the investigated conditions, with physics-based estimates.

Finally, a particularly promising direction concerns the systematic use of the global model to map the regimes of validity of the static approximation for molecular ions. Beyond the specific GyM operating conditions considered here, a parametric scan of the global model over a wider range of plasma densities and temperatures could be performed to quantitatively identify the threshold conditions below which the approximation breaks down. This would allow a more general assessment of where, and to what extent, the current SOLPS-ITER treatment of molecular ions can be trusted. While the static approximation is generally considered valid under typical tokamak SOL conditions, localized regions of reduced density may approach the regime in which the assumption becomes questionable. A dedicated investigation in this direction would help establish whether the limitations identified in this work are specific to LPDs or have broader implications for SOLPS-ITER simulations of tokamak-relevant scenarios. Future developments of the SOLPS-ITER molecular-ion modeling strategy could be pursued, with the global model serving as a valuable tool to guide and support this process.

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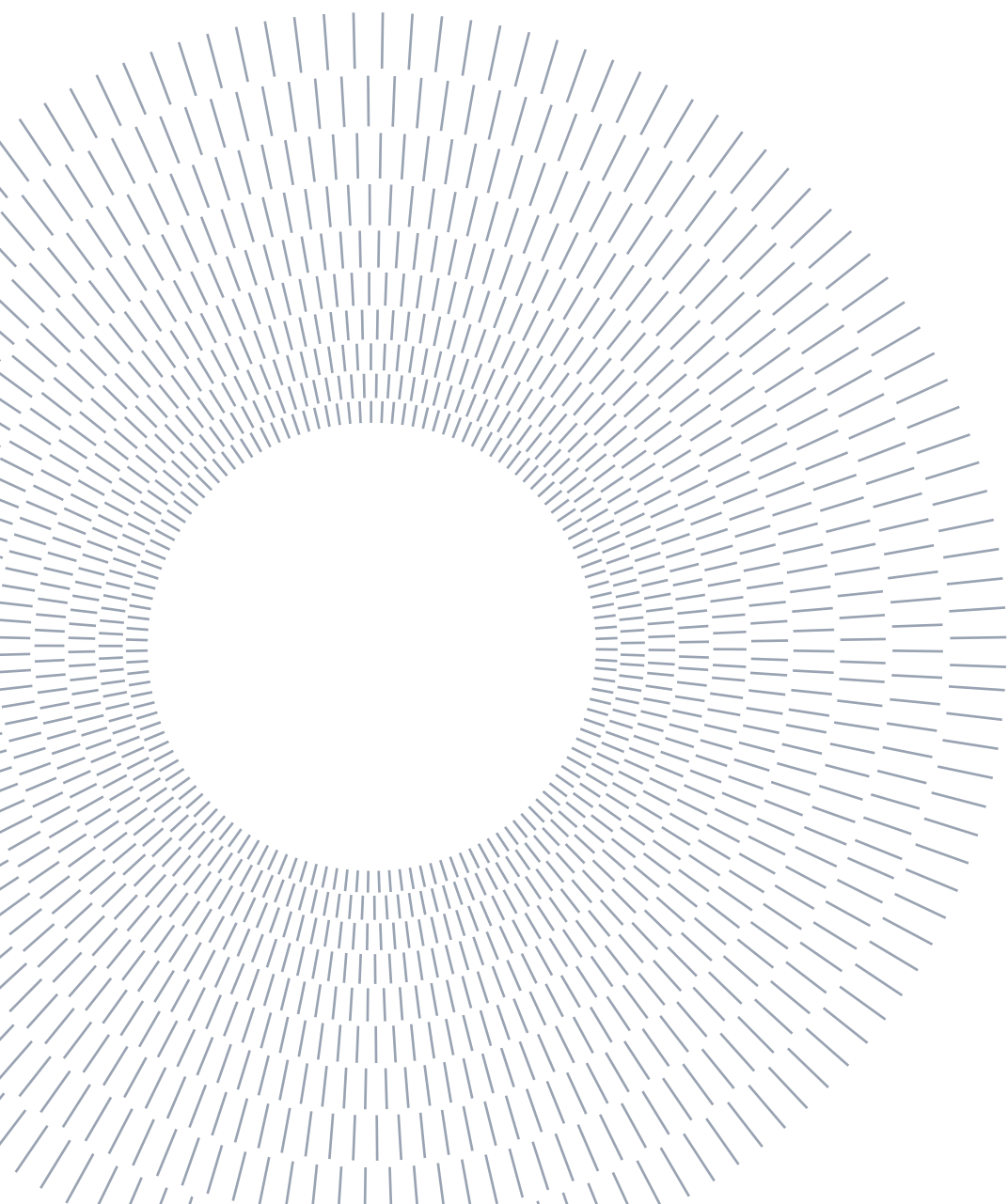
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