Validation of tungsten erosion and transport simulations in tokamaks

Henri Kumpulainen
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Henri Kumpulainen

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Abstract

This dissertation evaluates the validity and options for improvement of simulation codes in predicting tungsten erosion and transport in tokamaks, by code-code comparisons and validation against measurements from JET and ASDEX Upgrade experiments. Tungsten is a leading candidate as the plasma-facing material in magnetic confinement fusion power plants. However, W contamination of the fusion plasma is highly detrimental to reactor performance and impedes the attainment of viable power production. The ability to predict the erosion rate of W components and the resulting W density in the plasma is crucial for designing fusion reactors. The simulations studied in this thesis predict the sputtering of W atoms from plasma-facing components, their ionisation in the scrape-off layer, and the transport of W ions parallel and perpendicular to the magnetic field in the scrape-off layer, pedestal, and core plasma regions.

In this thesis, the predicted W erosion rate at the JET divertor targets is found to have a negligible impact on the W density in the main plasma due to efficient divertor screening. According to EDGE2D-EIRENE, DIVIMP, and ERO2.0 predictions, the W influx to the main plasma is predominately due to W sputtering near the low-field side divertor entrance due to energetic D atoms created by charge-exchange.

EDGE2D-EIRENE consistently predicts 30--40% lower W density in the main plasma compared to DIVIMP in both L-mode and H-mode plasmas. In this work, the difference is demonstrated to be mostly due to the bundling of the 74 W ionised charge states into 6 fluid species in EDGE2D-EIRENE. Integrated core-edge JINTRAC predictions agree with measurements of the main plasma W density in L-mode, indicating that both the DIVIMP and EDGE2D-EIRENE predictions are consistent with the experimentally inferred W density within a factor of 2.

Simulations of high-power type-I ELMy H-mode plasmas, using ERO2.0 for W erosion and transport in the edge plasma and JINTRAC with NEO for core W transport, predict the 2D poloidal W density profile in agreement with the inferred W density within the modelling uncertainties. Accurate predictions of the main plasma W density in type-I ELMy H-mode require thorough validation of the simulated ELM and edge transport barrier properties, as well as precise reproduction of the toroidal rotation frequency, and the ion temperature and density gradients in the main plasma.

Keywords fusion, tokamak, plasma, tungsten, sputtering, transport, simulation, validation

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Tiivistelmä
Tässä väittöskirjassa arvioidaan volframin eroosiot ja kulkeutumista tokamakeissa ennustavien simulointikoodien pätevyyttää ja kehityskohteita vertailemalla koodeja ja validoimalla ne JET- ja ASDEX Upgrade-kokeiden mitattuksilla. Volframi on johtava vaihtoehto magneettisen koosapidon fuusiovoimalaitosten seinämämatериалiksi. Fuusioplasman saastuminen volframilla on kuitenkin suureksi haitaksi reaktorin suorituskyvylle ja uhkaa kannattavan energiantuotannon saavuttamista.


Avainsanat
fuusio, plasma, tokamak, volframi, sputterointi, kulkeutuminen, simulaatio, validointi

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Preface

The research presented in this thesis was carried out at Aalto University during 2019–2023, including multiple research visits to Culham Centre for Fusion Energy, UK, and Forschungszentrum Jülich, Germany. I am most grateful to professor Mathias Groth, my thesis advisor and supervisor, for all the valuable time and effort dedicated to making this thesis project possible, and for the expertise and feedback which has helped me improve as a researcher. Connecting me with top experts from around the world has also been invaluable to me.

I greatly appreciate the time and expertise of Gerard Corrigan, Derek Harting, Florian Köchl, Juri Romazanov, and Francis Casson in tutoring me with setting up, executing, and interpreting simulations using state-of-the-art codes, and the answers they provided to my numerous technical questions.

The JET and ASDEX Upgrade contributors are thankfully acknowledged for providing measurement data and computational tools. A special thank you is expressed to Juuso Karhunen, Bart Lomanowski, Andrew Meigs, and Marco Sertoli.

I also thank all of my colleagues at Aalto University, CCFE, and FZJ for the very positive experience of working with you. In particular I would like to mention Sebastijan Brezinsek and Andreas Kirschner from FZJ, and fellow doctoral students Andreas Holm, Vladimir Solokha, and Roni Mäenpää from Aalto University for many insightful discussions and feedback.

Acknowledgement

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission
can be held responsible for them. The computational resources provided by the Aalto Science-IT project are gratefully acknowledged.

Espoo, April 24, 2023,

Henri Kumpulainen
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This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.


Author’s Contribution

Publication I: “Comparison of DIVIMP and EDGE2D-EIRENE tungsten transport predictions in JET edge plasmas”

The author performed the setup, troubleshooting, execution, post-processing, analysis, and interpretation of the EDGE2D-EIRENE and DIVIMP simulations. The author was also the main writer of the manuscript. M. Groth was the academic supervisor and secondary writer of the manuscript. M. Fontell and A.E. Jaervinen provided instructions and post-processing software for the DIVIMP simulations. M. Groth and A.E. Jaervinen conceived the research plan. M. Groth, G. Corrigan, and D. Harting provided instructions and feedback on the setup, post-processing, and interpretation of the EDGE2D-EIRENE simulations.

Publication II: “Validation of EDGE2D-EIRENE and DIVIMP for W SOL transport in JET”

The author performed the setup, execution, post-processing, analysis, and interpretation of the EDGE2D-EIRENE, DIVIMP, and JINTRAC simulations. The author was also the main writer of the manuscript. M. Groth was the academic supervisor and secondary writer of the manuscript. A.E. Jaervinen provided post-processing software for the DIVIMP simulations. G. Corrigan, D. Harting, and F. Koechl provided instructions and feedback on the setup, post-processing, and interpretation of the JINTRAC and EDGE2D-EIRENE simulations. B. Lomanowski provided post-processing software for synthetic diagnostics. A.G. Meigs and M. Sertoli analysed the experimental measurements.
Author's Contribution

Publication III: “ELM and inter-ELM tungsten erosion sources in high-power, JET ITER-like wall H-mode plasmas”

The author performed the setup, execution, post-processing, analysis, and interpretation of the EDGE2D-EIRENE, JINTRAC, and ERO2.0 simulations. The author was also the main writer of the manuscript. M. Groth was the academic supervisor and secondary writer of the manuscript. S. Brezinsek planned, coordinated, and supervised the experiments of the reference plasma scenario. M. Groth, S. Brezinsek, and the author conceived the research plan. G. Corrigan, D. Harting, and F. Koechl contributed to the setup and post-processing of the JINTRAC and EDGE2D-EIRENE simulations. B. Lomanowski provided post-processing software for synthetic diagnostics. L. Frassinetti, A.G. Meigs, and J. Karhunen analysed and processed the measurement data. M. O’Mullane provided atomic data for the ERO2.0 simulations. J. Romazanov provided instructions, software updates, and pre- and post-processing tools for the ERO2.0 simulations.

Publication IV: “ERO modelling of net and gross erosion of marker samples exposed to L-mode plasmas on ASDEX Upgrade”

The author supervised the setup, initial execution, and post-processing of the ERO simulations, solved the technical issues encountered using the ERO code, contributed to the interpretation and analysis of the results, and carried out the majority of the final published ERO simulations and post-processing. A. Hakola carried out planning, analysis, and interpretation of the experiments and ERO simulations, and was the main writer of the manuscript. A. Keitaanranta performed the initial ERO simulations and post-processing. A. Hakola and M. Groth provided academic supervision. A. Lahtinen and M. Balden carried out analysis of the marker samples. J. Likonen coordinated the plasma experiments. M. Cavedon performed the spectroscopic measurements. K. Krieger prepared and supervised the plasma experiments. M. Airila provided technical counselling and pre-processing software for the ERO simulations.
1. Introduction

1.1 Thermonuclear fusion

Thermonuclear fusion refers to the merging of atomic nuclei brought sufficiently close together at a high temperature, resulting in transmutation from lighter to heavier elements. Fusion reactions release or consume energy equivalent to the difference in the nuclear binding energy of the initial and produced nuclei. The energy released by thermonuclear fusion reactions is what causes the stars to shine. Fusion energy produced by the Sun is the main energy source of life on Earth, both directly by mechanisms such as photosynthesis, or indirectly by enabling the growth of producers in the ecosystem and by driving wind, rainfall, and many other phenomena.

Collisions between atomic nuclei are far more likely to scatter the nuclei apart than to fuse them together, even if the nuclei carry the kinetic energy required to overcome their electrostatic Coulomb repulsion. For this reason, producing more fusion energy than is needed to heat the nuclei is only possible if the nuclei are confined until their repeated collisions yield a sufficient rate of fusion before their energy is lost to the environment. If the temperature and density of the nuclei and the energy confinement time are sufficiently high, and the elements and isotopes are favorable for fusion, a self-sustaining fusion process can be achieved. The state in which the self-heating due to released fusion energy overcomes the total energy loss rate is called ignition. An ignited plasma continues to release energy without requiring external power input for as long as the temperature, density, and energy confinement of the fusion fuel are within the ignition criteria. The most favourable fuel for ignition, in terms of the highest fusion reactivity at the lowest required temperature (Fig 1.1), is a mix of the hydrogen isotopes deuterium (D) and tritium (T):

\[
^2_1\text{D} + ^3_1\text{T} \rightarrow ^4_2\text{He} (3.5 \text{ MeV}) + ^1_0\text{n} (14.1 \text{ MeV}) \quad (1.1)
\]
The requirement for ignition is more formally quantified as the Lawson criterion [2] for the minimum product of density and confinement time as a function of temperature. The criterion was later reformulated as a triple product of density $n$, temperature $T$, and energy confinement time $\tau_E$, with a minimum value for D-T fusion at $T \approx 14$ keV (Fig. 1.2):

$$nT\tau_E \geq 5 \cdot 10^{21} \text{ keV s m}^{-3}$$  \hspace{1cm} (1.2)

Net electricity production using fusion does not necessitate ignition. A sufficient condition is that the electric power harnessed from the reactor exceeds the electric power consumed by the plasma confinement, heating, and other systems required to operate the reactor. The ratio of produced to consumed electrical power $Q_{\text{total}}$ is a figure of merit for the efficiency of the power plant. For the purposes of studying fusion performance in devices which are not optimised for the electrical efficiency of power conversion, heating, and confinement systems, a more relevant figure of merit is the fusion gain $Q_{\text{plasma}}$, defined as the ratio of produced thermal fusion power to external heating power deposited in the plasma. $Q_{\text{plasma}} > 1$ is a prerequisite of $Q_{\text{total}} > 1$. 

![Figure 1.1. Reaction rates of selected fusion reactions as a function of the ion temperature [1].](image-url)
1.1.1 Approaches to fusion power

Stars have a high energy confinement time as a result of their very large volume, and a high density due to strong gravity, neither of which is a viable option in a fusion power plant on Earth. Despite those advantages, the volumetric fusion power density of solar-mass stars is impractically low for a power plant. Hence, feasible fusion power designs aim for temperatures at least an order of magnitude higher than in the core of the Sun, to reach a higher $Q_{\text{plasma}}$ at a given triple product and to obtain a useful rate of fusion power in a device not impractically large.

Artificial ignition of a fusion plasma was first achieved in 1952 by heating and compressing liquid deuterium with the detonation of a nuclear fission bomb [3], however a significant fraction of the energy released by thermonuclear weapons is in the form of a highly destructive pressure wave, which is uncontrollable after detonation and poorly suited for electricity production. Alternative methods to initiate fusion are required for safe and sustainable use inside a power plant.

Inertial confinement fusion (ICF) research aims to miniaturise the fusion bomb to small pellets for power production, while replacing the fission primer detonation with laser-induced X-ray radiation to heat and compress the plasma. The first ignition of a fusion plasma without nuclear weapons was achieved in 2021 by inertial confinement in the National Ignition Facility (NIF) [4]. However, ICF has the inherent drawback that each
pellet must be separately prepared and heated to ignition conditions, as opposed to a steady-state plasma continuously producing energy with little to no external heating. Therefore, reaching ignition conditions in an ICF device does not imply $Q_{\text{plasma}} > 1$. Indeed, the first NIF experiment which reached ignition had a $Q_{\text{plasma}}$ of 0.72, and the duration of the implosion was a fraction of a nanosecond [4]. In 2022, NIF exceeded $Q_{\text{plasma}} > 1.5$, however the low energy efficiency of the laser results in $Q_{\text{total}} < 0.01$, and increasing the implosion frequency by several orders of magnitude for viable power production remains an unsolved challenge [5].

Another approach to fusion power is to confine the plasma using magnetic fields, called magnetic confinement fusion (MCF). MCF devices typically operate at many orders of magnitude lower densities and higher energy confinement times than ICF devices. The leading early MCF concepts in the 1950s were cylindrical devices based on a mechanism called the plasma pinch, also occurring in lightning strikes, in which a high electric current induces a magnetic field and compresses the plasma. Such concepts achieved little to no fusion power due to plasma instabilities as well as poor energy and particle confinement. Later the focus of research shifted to magnetic geometries in which field lines form closed surfaces, improving the confinement, and plasmas with lower electric currents, less susceptible to current-driven instabilities.

1.2 Tokamak

A tokamak is a device which confines hot plasma in a toroidal vacuum chamber using a combination of magnetic field coils and an electric current induced in the plasma (Fig. 1.3). The superposition of toroidal and poloidal magnetic fields, created by poloidal field coils and a toroidal plasma current respectively, results in helical magnetic field lines which form closed magnetic flux surfaces nested within one another. The magnetic field reduces the transport of electrons and ions across the flux surfaces, making it possible to sustain fusion-temperature plasmas without destroying the vacuum vessel. Common methods of heating the plasma to fusion temperatures include neutral beam injection (NBI) in which ions are accelerated using an electric field, neutralised to atoms, and these atoms injected into the plasma; and electron and ion cyclotron resonance heating (ECRH and ICRH respectively) in which electromagnetic waves emitted by an antenna are absorbed by the plasma. The tokamak is thus far the most successful approach to MCF in terms of achieved fusion power (16.1 MW) and $Q_{\text{plasma}}$ (0.64) [6], although order-of-magnitude improvement is still required for feasible power production.

Based on experimentally established parameter scaling laws for fusion performance, it is estimated that a scaled-up version of existing tokamaks
with a major radius of 9 metres is capable of reaching $Q_{\text{plasma}} > 40$ and $Q_{\text{total}} > 1$, and could be built using proven technology and knowledge [7]. However, there remain open research questions regarding other requirements on a fusion power plant, such as achieving a viable reactor lifespan, predicting and mitigating plasma disruptions, controlling the heat exhaust to protect the plasma-facing components from damage, demonstrating adequate production of tritium fuel, and cost optimisations for economic viability. The ITER project [8] aims to address many of these questions, and demonstrate the engineering viability of fusion power, by building and operating a tokamak designed to reach $Q_{\text{plasma}} = 10$. As of late 2022, the ITER tokamak is undergoing assembly with progress towards its first plasma at 78% [8].

1.2.1 Scrape-off layer

Despite the efforts to prevent the hot plasma from reaching the chamber walls, Coulomb scattering and electromagnetic drifts inevitably cause transport of particles and heat from one flux surface to another. Eventually the electrons and ions are transported to open flux surfaces which intersect the walls. The set of open flux surfaces around the main plasma constitutes a region called the scrape-off layer (SOL), in which particles escaping the main plasma are able to reach the wall along magnetic field lines (Fig. 1.4). The boundary between open and closed flux surfaces is called the separatrix. The locations in which the separatrix intersects wall surfaces are called strike points.

While every tokamak plasma has a separatrix and a SOL, it is possible to
construct magnetic geometries in which the plasma-wall contact occurs far away from the closed flux surfaces, enabling lower plasma temperatures at the walls and reduced impurity concentrations in the core plasma. By adding a second toroidal current outside the plasma, the induced poloidal magnetic field reaches zero at a location called the X-point (Fig. 1.4). The X-point separates the main plasma from another region called the private flux region (PFR), in which the flux surfaces intersect the wall but do not envelop the main plasma as they do in the SOL. This magnetic field arrangement is called the divertor configuration, as the heat and particle flux parallel to SOL flux surfaces is diverted from the main chamber into designated parts of the wall called divertor targets. The two major advantages of creating distance between the confined plasma and the plasma-wall contact are that i) the plasma at the walls can be much colder than at the last closed flux surface, protecting the walls from damage, and ii) eroded wall material has a much lower probability of contaminating the main plasma.

1.2.2 Plasma confinement modes

When the heat flux carried by the plasma across the separatrix exceeds a configuration-specific threshold value, a transition from lower to higher energy confinement is observed [10]. The states of lower and higher confinement are called low-confinement mode (L-mode) and high-confinement mode (H-mode) respectively. The improvement of energy confinement is due to the formation of a transport barrier near the separatrix, in which turbulent heat and particle losses are suppressed by electric field shearing [11]. The reduced turbulence leads to the build-up of steep electron density and temperature gradients across the transport barrier, creating a radial plasma pressure profile with a shape resembling a pedestal (Fig. 1.5). The edge plasma region inside the transport barrier is called the pedestal. H-mode enables a significantly higher triple product compared to L-mode at a given magnetic field $B_t$ and plasma current $I_p$, which is required for economical fusion performance.

H-mode plasmas often involve instabilities known as edge-localised modes (ELMs), which cause quasi-periodic bursts of particles and heat from the confined plasma to be expelled into the SOL. The most severe type of ELMs is called the type-I ELM, generally observed in plasmas significantly above the H-mode power threshold. Type-I ELMs in reactor-scale devices are foreseen to damage the plasma-facing components as they outmatch the heat tolerance limits of any known material. However, the highest steady and sustainable fusion performance in current tokamaks is obtained in the type-I ELMy regime [12]. Thus, tokamaks designed for electricity production must either employ reliable means to mitigate the heat load caused by type-I ELMs or operate in a lower-performance plasma
**Figure 1.4.** Poloidal cross-section of the JET tokamak. The inner contour of the plasma-facing components is shown in red. Selected open and closed magnetic flux surfaces from JET pulse number (JPN) 81472 at 9 seconds are indicated by dark blue lines. The main plasma region is coloured yellow, the SOL is light blue, and the PFR is light green.
Introduction

The erosion rate of plasma-facing components may increase by orders of magnitude during type-I ELMs, creating major sources of plasma impurities. Conversely, convective outward transport of particles at the ELM onset reduces the impurity content in the edge of the main plasma. This thesis studies the behaviour of impurities in the relatively quiescent L-mode as well as in the alternating ELM and inter-ELM phases of type-I ELMy H-mode plasmas.

1.3 Scope of the thesis

This thesis addresses the following research questions:

1. How accurately can simulations predict the erosion rate of tokamak plasma-facing components?

2. How accurately can simulations predict the impurity density in the confined plasma?

3. Which model input parameters and model assumptions induce significant uncertainty in the impurity predictions?
4. What are the advantages and shortcomings of each of the studied physics models in practice, and how could their predictive capabilities be improved?

Table 1.1 describes how each publication contributes to the research topics of the thesis, and which simulation tools, tokamak, and confinement modes were studied in each publication.

<table>
<thead>
<tr>
<th>Publication</th>
<th>Research topic</th>
<th>Simulation tools</th>
<th>Tokamak</th>
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Table 1.1. Summary of publications by research topic, applied simulation tools, tokamak in which the experiments were carried out, and studied plasma confinement modes. The simulation tools and their physics models are described in chapter 4.

Chapter 2 describes the theory and mechanisms of impurity erosion and transport in tokamak plasmas. Chapter 3 introduces the simulation tools, their physics models and assumptions, and the setup of the simulations. Chapter 4 contains an overview of plasma impurity diagnostics and the methodology of inferring the impurity density and erosion rate from measurements. Chapter 5 presents the main results on the above-mentioned research topics, based on publications I-IV. Chapter 6 concludes the thesis.
2. Impurity erosion and transport processes in tokamaks

Figure 2.1. Schematic of the sputtering of W atoms (dark green) and W ion transport parallel (blue arrows) and perpendicular (purple arrows) to the magnetic field in the SOL (light blue), pedestal (yellow) and core (orange) regions in a poloidal cross-section of a tokamak with a W divertor and a Be main chamber.
This chapter discusses the physical processes related to plasma-surface interactions and the transport theory of impurities in tokamak plasmas (Fig. 2.1).

### 2.1 Plasma-surface interactions

#### 2.1.1 Sputtering

Sputtering refers to the erosion of solid material surfaces due to an incident flux of fuel or impurity ions or atoms (Fig. 2.2). Sputtering processes can be classified as physical or chemical sputtering. In physical sputtering, an impacting ion or atom transfers sufficient kinetic energy and momentum to the surface to break inter-atomic chemical bonds, ejecting one or more atoms away from the surface. In chemical sputtering, surface atoms form chemical bonds with the incident particles, creating molecules which are no longer tightly bound to the surface.

The ratio of released surface atoms to incident ions is called the sputtering yield. Physical sputtering yields vary greatly depending on the energy, mass, and impact angle of the incident ions, as well as on the surface binding energy and mass of the surface atoms (Fig. 2.3). Databases of the physical sputtering yields are created based on empirical models fitted to measurements of sputtering [13] and based on molecular dynamics (MD) or binary-collision approximation (BCA) simulations [14]. Unlike physical sputtering, chemical sputtering depends strongly on the surface temperature and the chemical properties of the incident and surface materials.
Figure 2.3. Sputtering yield of a) W by H, D, T, Be, and W projectiles at a 60° impact angle and b) W by D and Be projectiles at selected impact angles as a function of impact energy, calculated by the BCA code SDTrimSP (markers) and interpolated using thin plate spline interpolation (solid and dashed lines).
2.1.2 Choice of plasma-facing materials

This thesis studies the sputtering of the plasma-facing materials beryllium (Be) and tungsten (W) used in the JET ITER-like wall (JET-ILW) [15] and ASDEX Upgrade (all W) [16]. The same materials are also relevant to the future fusion devices ITER [15] and DEMO [7]. JET-ILW and ITER have Be limiters in the main chamber and a W divertor, whereas ASDEX Upgrade and the current design of DEMO have W components in both the main chamber and the divertor. The erosion of W under typical scrape-off layer plasma conditions is dominated by physical sputtering, whereas chemical sputtering is negligible in comparison [17]. The majority of Be erosion is also physical sputtering, with a contribution of up to one-third chemically-assisted physical sputtering at surface temperatures lower than 700 K [18].

2.1.3 Role of the sheath

A solid surface exposed to a plasma of no net electric charge, and of electron temperature $T_e$ of similar order of magnitude or greater than ion temperature $T_i$, gains a negative potential due to the far higher thermal velocity of electrons compared to ions. The negatively charged wall surface repels electrons and attracts ions, equalising the current densities of electrons and ions into the surface. Consequently, a micrometre-scale layer of charge imbalance known as the Debye sheath is formed in the plasma adjacent to the surface. For a magnetic field which is non-perpendicular with respect to the surface, a magnetic pre-sheath [19], also called the Chodura sheath, is formed. The magnetic pre-sheath is electrically quasineutral, meaning that the densities of free positive and negative charges are approximately equal at each location. The magnetic pre-sheath extends several times further from the surface than the Debye sheath. The combined effect of the electric field in the Debye sheath and the relatively weaker electric field in the magnetic pre-sheath increases the impact energy of each ion by approximately $3Z_i k_B T_e / e$ [20]. Due to the sensitivity of the sputtering yields to the impact energy, the ion charge state and the local electron temperature are crucial parameters in determining the sputtering rate due to ions.

2.1.4 Scrape-off layer regimes

The plasma conditions in the SOL are classified into three regimes based on plasma-surface interactions: the low-recycling regime, the high-recycling regime, and the detached regime [21]. In the low-recycling regime, the SOL is low-density and nearly isothermal along the magnetic field. For typical low-recycling JET L-mode scrape-off layer conditions, $n_e < 10^{19} \text{ m}^{-3}$
Impurity erosion and transport processes in tokamaks

Figure 2.4. Effective rate coefficients of relevant atomic processes in a D plasma with W impurities, as functions of electron temperature, assuming an electron density of $10^{20} \text{ m}^{-3}$ [23].

and $T_e > 40$ eV. The ion flux $\Gamma_i$ to wall surfaces is approximately linearly proportional to the "upstream" main chamber SOL density $n_u$ and to $\sqrt{T_i}$. Ions reaching the wall are recycled back into the plasma as electrically neutral atoms or molecules which have a high ionisation mean-free path due to the low electron density.

In the high-recycling regime, the electron density near the surfaces is sufficiently high that the vast majority of recycled neutral particles are re-ionised close to the surface, forming an ionisation front in which the ions rapidly circulate between the surface and the plasma. For a typical high-recycling JET L-mode, $10^{20} \text{ m}^{-3} < n_e < 2 \cdot 10^{20} \text{ m}^{-3}$ and $2 \text{ eV} < T_e < 10$ eV at the divertor targets. As the sink and the primary source of ions are adjacent to each other, the (convective) plasma flow from the main chamber is reduced and the heat transfer is largely conductive. Conductive heat transfer necessitates a parallel-B temperature gradient, most significant at low divertor temperatures, as the conductive heat flux density is $q_\parallel = -\kappa T_5/2 dT/ds$ [22], with $\kappa \approx 2000$ for electrons and $\kappa \approx 60$ for deuterium ions. Assuming constant pressure along field lines, the ion and electron temperatures at the sheath entrance are thus strongly decreasing functions of $n_u$: $T_e, T_i \propto n_u^{-2}$ [21]. The ion flux to the divertor targets is proportional to $n_u^2$ and the electron density at the sheath entrance is proportional to $n_u^3$ [21].

As the upstream density is further increased, eventually the heat flux density into the divertor is too low to ionise all of the recycled neutral particles near the targets. The ionisation front detaches from the target and extends further upstream. Correspondingly, the ion flux to the target
reaches a maximum value and starts decreasing as a function of \( n_u \) [21]. The \( n_u \) value of maximum \( \Gamma_i \) is called the onset of detachment. In the detached regime with typical JET L-mode values \( n_u > 2 \cdot 10^{19} \, \text{m}^{-3} \) upstream, \( n_e \lesssim 2 \cdot 10^{20} \, \text{m}^{-3} \) and \( T_e < 1 \, \text{eV} \) at the targets, a layer consisting of mostly atoms and molecules exists between the plasma and the targets, further reducing the momentum and heat flux carried by the plasma to the targets via friction as well as atomic and molecular-assisted volume recombination and charge-exchange reactions (Fig. 2.4). The electron temperature near the targets is of the order of 1 eV or lower. The detached regime is ideal for conforming to the heat tolerance limits of plasma-facing materials and achieving minimal sputtering. However, the options for reaching detachment at high SOL heat fluxes require compromises in fusion performance and/or less efficient use of magnetic volume, which poses a challenge to fusion reactor design [24].

### 2.1.5 Neutral particle interactions with surfaces

The magnetic field, which confines ions and electrons to helical orbits around magnetic field lines, does not confine neutral particles such as atoms, molecules, photons, and neutrons. Thus, all surfaces with a direct or reflected line-of-sight to the plasma receive some incident particle and energy flux due to atomic processes and radiation from the plasma. Out of the neutral particle species in tokamak plasmas, fuel atoms (isotopes of hydrogen) with energy above the sputtering threshold are generally the largest cause of erosion, which may occur even on surfaces which are not in plasma contact. The momentum carried by photons is too low to cause physical sputtering, and neutrons typically deposit their energy too deep within the material to sputter. Plasmas which produce molecules at a high rate tend to be too cold for physical sputtering of heavy elements.

Fuel atoms are released from wall surfaces primarily due to reflections and recycling, and created in the plasma volume due to dissociation of molecules, recombination of ions with electrons, and charge-exchange (CX) reactions between ions and atoms or molecules (Fig. 2.2). The typical energies of such atoms, sorted by origin from lowest to highest energy, are on the order of the wall temperature (0.05 eV) for recycled atoms, a few eV for dissociation and recombination products, the local ion temperature (1 to 1000 eV) for charge-exchange atoms, and a significant fraction of the ion impact energy (5 to 3000 eV) for wall reflections.

In the case of tungsten plasma-facing surfaces, the sputtering threshold is generally exceeded by only a small fraction of the incident atoms. Sputtering due to wall reflections can be virtually eliminated by reducing the ion and electron temperature at the divertor (or limiter) targets. However, fusion-relevant plasmas in existing and planned tokamaks have ion temperatures ranging from several hundred to thousands of eV in the edge of
the main plasma, exceeding the D-on-W sputtering threshold. Thus, atoms undergoing CX in the main plasma produce atoms with sufficient energy to cause W erosion. During ELMs, even the scrape-off layer ion temperature may exceed the W sputtering threshold, greatly increasing the fraction of atoms which contribute to CX sputtering of W.

Impurity ions with bound electrons also augment the production of CX atoms from thermal ions. However, the vast majority of the CX sputtering of W typically occurs due to fuel atoms rather than impurities (Publication II). Besides fuel ions being the most abundant ion species, an even more significant reason to the low CX erosion by impurities is that CX atoms are produced from singly-charged ions, and singly-charged impurity ions are likely to re-ionise to higher charge states before they reach energies above the W sputtering threshold. The self-sputtering of impurities is thus typically dominated by ions as opposed to atomic impurities.

2.1.6 Deposition and reflection

When ions or atoms collide with a solid surface, they are either reflected back with some fraction of their impact energy or deposited onto the surface. In addition, the surface impact may result in sputtering (section 2.1.1). The fraction of reflected particles, also called the reflection coefficient, as well as the energy and angular distributions of the reflections, can be calculated using BCA or MD codes similarly to the sputtering coefficients [14]. Due to the overabundance of electrons on plasma-wetted surfaces (section 2.1.3), reflecting ions are likely to undergo surface recombination and become atoms.

Sputtered atoms which are ionised close to a surface in such a manner that their Larmor orbit intersects the surface, are promptly redeposited before completing a single orbit. Atoms which are ionised close to a plasma-wetted surface but not promptly redeposited, are likely to be locally redeposited near the ionisation location due to the combined effect of plasma flow towards the surface (section 2.2.3) and the electric field of the magnetic pre-sheath (section 2.1.3). Atoms sputtered from regions in which the electron density or temperature is too low to efficiently ionise near the surfaces, and atoms which for other reasons penetrate sufficiently deep into the plasma before ionising, have a higher probability of migrating to a different plasma-facing component. Local erosion and deposition has been observed to create small valleys and ridges on wall areas continuously receiving the highest heat and particle fluxes [25], whereas migration of eroded material into low-erosion regions results in net deposition and accumulation of deposit layers [26].

Deposited gaseous elements, such as hydrogen, helium, or neon, tend to have a saturation point beyond which the surface content of deposited atoms does not significantly increase as a function of incident fluence.
Once saturation is reached, the rate of deposition approximately equals the rate of atoms or molecules recycled from the surface. Typical energies of recycled particles are of the same order as the surface temperature. Solid materials such as beryllium and tungsten typically accumulate as deposit layers on top of the surface, as opposed to recycling.

In net deposition regions, recycling may be reduced due to atoms and molecules becoming trapped within the accumulating deposit layers. This process is called co-deposition. Tritium co-deposition with eroded wall materials may pose a radiological safety hazard in planned fusion reactors [27]. Fuel retention due to co-deposition can be mitigated by choosing plasma-facing materials with high resilience against erosion and therefore low deposition rate. Dedicated plasma discharges for wall conditioning may also be carried out to clean deposit layers of retained fuel.

Additionally, ions and atoms impacting a surface with sufficiently high energy are implanted within the bulk material and retained beneath the surface layers. Implantation can be mitigated by operating plasmas at lower SOL temperature.

### 2.1.7 Material mixing

Ions of different elements being deposited onto a wall component affects the surface material composition, and thereby also alters the reflection, sputtering, and recycling properties of the surface. Even in regions of net erosion, without any accumulation of deposit layers, the surface concentrations of deposited impurities and the original wall materials tend towards a dynamic equilibrium which differs from a pure surface.

Accounting for the surface mixing of materials, and the resulting re-erosion of deposited impurities, is particularly important when a re-eroded impurity species is the dominant cause of erosion of heavier elements. A notable example of such mixing is Be ions being the largest contributor to L-mode and inter-ELM erosion of W in the JET-ILW divertor [17]. For every Be ion transported from the main chamber SOL into the divertor, there are multiple Be atoms re-eroded from the divertor targets and ionised in the SOL, because the typical distance travelled by an eroded impurity before redeposition is many times shorter than the dimensions of the net erosion region [25]. Whether reflections are considered or not, the majority of Be ions incident on the divertor targets are therefore deposited and re-eroded from the divertor, likely multiple times. Neglecting the re-eroded Be would cause the estimated W erosion by Be ions to be several times too low.
2.2 Impurity transport

The transport of a charged particle in an electromagnetic field is described by the Lorentz force:

$$\frac{d\vec{v}}{dt} = \frac{q}{m} \vec{E} + \vec{v} \times \vec{B} \quad (2.1)$$

In the absence of other forces, ions and electrons accelerate along electric field lines and gyrate in helical orbits (Larmor orbits) around magnetic field lines. However, obtaining the complete microscopic description of the electric and magnetic fields requires simultaneously following the path of every ion and electron in the system, which is computationally very expensive and tends to limit the simulation to impractically small volumes in the case of a fusion plasma. The gyrokinetic approximation, averaging the particle motion over the Larmor orbits, reduces the dimensionality of the problem by one, however the computational cost remains significant for large systems. Additionally, the gyrokinetic approximation is not applicable on length scales smaller or equal to the gyroradius, for example in prompt redeposition studies.

In practice, a more useful approach than tracking every particle individually is to follow the collective behaviour of the particle distribution using stochastic differential equations. The distribution of a particle species $\alpha$ is described by the kinetic distribution function $f_\alpha(\vec{r}, \vec{v}, t)$, yielding the expected fraction of particles which are located at each point in space $\vec{r}$ and have a velocity vector $\vec{v}$ at each time $t$. The equation describing the time evolution of the distribution function is called the Fokker-Planck equation [28]:

$$\frac{\partial f_\alpha}{\partial t} + \frac{\partial}{\partial \vec{r}} (\vec{v} f_\alpha) + \frac{\partial}{\partial \vec{v}} (\frac{\partial \vec{v}}{\partial t} f_\alpha) = \sum_\beta C_{\alpha \beta}(f_\alpha, f_\beta) \quad (2.2)$$

The collision operator $C_{\alpha \beta}$ on the right-hand side of the Fokker-Planck equation is a sum of terms describing particle collisions between the species $\alpha$ and each of the species $\beta$ present in the plasma.

2.2.1 Trace-impurity approximation

Assuming $\alpha$ is a minority species with a negligible impact on the electromagnetic fields and on the distribution of other species, the Fokker-Planck equation can be decoupled into an equation for the background distribution $f_\beta$, independent of the trace-impurity species $\alpha$, and another equation for $f_\alpha$ as a function of the background distribution function. The collision operator $C_{\alpha \beta}$ can then be written as a sum of drift and diffusion terms [29]:

$$C_{\alpha \beta}(f_\alpha, f_\beta) = - \sum_i \frac{\partial}{\partial v_i} (K_i f_\alpha) + \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial v_i \partial v_j} (D_{ij} f_\alpha) \quad (2.3)$$
The drift vector $K_i$ and the diffusion tensor $D_{ij}$ represent the collective convective transport and stochastic diffusive transport respectively, and are defined as:

$$K_i = \left(1 + \frac{m_\alpha}{m_\beta}\right) \Lambda \frac{\partial}{\partial v_i} \left( \int \frac{f_\beta(\vec{v})}{|\vec{v} - \vec{v}'|} d\vec{v}' \right)$$

$$D_{ij} = \Lambda \frac{\partial^2}{\partial v_i \partial v_j} \left( \int |\vec{v} - \vec{v}'| f_\beta(\vec{v}') d\vec{v}' \right)$$

$$\Lambda = \frac{\lambda Z_\alpha^2 Z_\beta^2 e^4 n_\beta}{4\pi \varepsilon_0^2 m^2}$$

$m_\alpha$ and $m_\beta$ are the masses of the trace-impurity and background species respectively, $Z_\alpha$ and $Z_\beta$ are their charge states, $n_\beta$ is the background ion density, $e$ is the elementary charge, $\lambda$ is the Coulomb logarithm [30], and $\varepsilon_0$ is the vacuum permittivity.

### 2.2.2 Fluid approximation

For many practical applications, macroscopic quantities such as density, temperature, particle and heat fluxes, and net flow velocity are relevant, whereas detailed knowledge of the velocity distribution is not necessary. In such cases, the computational complexity of the kinetic equations can be greatly reduced by integrating the distribution function over all dimensions in velocity space. Instead of solving for a 7-dimensional distribution function (3 dimensions for space, 3 for velocity, and 1 for time), the problem is reduced to solving 4-dimensional field quantities as functions of space and time only. This description treats each particle species as a continuous fluid moving at a flow velocity $\vec{v}_\alpha(\vec{r}, t)$ as opposed to a distribution of particles $f_\alpha(\vec{r}, \vec{v}, t)$ moving in every direction at every point in space and time. A Maxwellian distribution is implicitly assumed, implying that additional corrective terms may be necessary for the fluid equations to reproduce the predictions of the Fokker-Planck equation in non-Maxwellian plasmas, in which external sources or perturbations are significant compared to equilibration via particle collisions.

The dimensionality of the fluid transport problem can be further reduced in special cases with symmetries in space or time. For example, a steady-state solution is a function of the spatial dimensions only, a toroidally symmetric plasma can be described by 2 spatial dimensions instead of 3, and assuming both toroidal and poloidal symmetry allows simplifying the geometry to a 1D radial profile. Each of the eliminated dimensions may lower the computational cost by several orders of magnitude, however the symmetries are not guaranteed to be valid assumptions in the general case discussed in this chapter.
The density, momentum, pressure, and heat flux of the fluid can be expressed as velocity moments of the distribution function:

\[ n_\alpha(\vec{r},t) = \int f_\alpha(\vec{r},\vec{v},t)d\vec{v} \]  
(2.7)

\[ n_\alpha(\vec{r},t)\vec{v}_\alpha(\vec{r},t) = \int \vec{v}f_\alpha(\vec{r},\vec{v},t)d\vec{v} \]  
(2.8)

\[ p_\alpha(\vec{r},t) = \int \vec{v}^2f_\alpha(\vec{r},\vec{v},t)d\vec{v} \]  
(2.9)

\[ \vec{q}_\alpha(\vec{r},t) = \int \vec{v}^3f_\alpha(\vec{r},\vec{v},t)d\vec{v} \]  
(2.10)

The plasma fluid equations are obtained from conservation laws for particles, momentum, and energy [31]:

\[ \frac{\partial}{\partial t}n_\alpha + \nabla \cdot (n_\alpha \vec{v}_\alpha) = S_\alpha \]  
(2.11)

\[ m_\alpha n_\alpha \left( \frac{\partial}{\partial t} + \vec{v}_\alpha \cdot \nabla \right) \vec{v}_\alpha = -\nabla \cdot \vec{P}_\alpha + Z_\alpha n_\alpha (\vec{E} + \vec{\nabla} \times \vec{B}) + \vec{F}_\alpha \]  
(2.12)

\[ \frac{3}{2} m_\alpha \left( \frac{\partial}{\partial t} + \vec{v}_\alpha \cdot \nabla \right) p_\alpha = -\frac{3}{2} p_\alpha \nabla \cdot \vec{v}_\alpha - \sum_{ij} (P_\alpha)_{ij} \frac{\partial (v_\alpha)_j}{\partial r_i} - \nabla \cdot \vec{q}_\alpha + W_\alpha \]  
(2.13)

\( S_\alpha \) is the particle source density of species \( \alpha \), \( P_\alpha \) is the stress tensor, \( \vec{F}_\alpha \) is the momentum source density, and \( W_\alpha \) is the energy source density. The source terms \( S_\alpha, \vec{F}_\alpha, \) and \( W_\alpha \) include the sources and sinks due to collisions and reactions with other particle species, as well as any external sources and sinks.

In principle, there are infinitely many fluid equations for each plasma species if also the higher-order velocity moments beyond the heat flux are included. Each conservation law for the \( n \)th-order velocity moment includes a term which depends on the \((n+1)\)th order velocity moment. This is referred to as the closure problem. In real-world applications, the closure problem can be addressed by truncating the higher-order moments or by assigning some value or formula to the highest-order moment in the last fluid equation. For example, the EDGE2D edge fluid plasma code uses a closure scheme truncated at 21 moments [32].

### 2.2.3 Parallel-B impurity transport mechanisms

Combining the trace-impurity approximation with a multi-fluid description of the plasma, a tractable force balance model can be derived for calculating the impurity density \( n_Z \) along magnetic field lines [33]:

\[ n_Z m_Z \left( \frac{\partial v_z}{\partial t} + \frac{1}{2} \frac{\partial v_z^2}{\partial s} \right) + \frac{\partial p_z^2}{\partial s} - n_Z Z eE - n_Z m_Z \frac{v - v_z}{\tau_z} \]

\[ - \alpha_z n_Z \frac{\partial (kT_e)}{\partial s} - \beta_z n_Z \frac{\partial (kT_i)}{\partial s} = (S_{ion} + S_{recomb} + S_{ext}) m_Z v_z \]  
(2.14)
The left-hand side terms are, in order from left to right, the acceleration and inertia of parallel-B impurity flow, the impurity pressure gradient force, the electrostatic force, the friction force, and the electron and ion temperature gradient forces. $m_z$, $v_z$, $p_z$, and $Z$ are respectively the mass, velocity, pressure, and charge number of the impurity species. $v$ is the velocity of fuel ions, and $s$ refers to distance along magnetic field lines. $S_{\text{ion}}$ includes the ionisation source from charge state $Z-1$ and the sink due to ionisation into state $Z+1$, and $S_{\text{recomb}}$ is the corresponding recombination source from $Z+1$ and sink into $Z-1$. $S_{\text{ext}}$ contains the external sources and sinks, such as additional terms to account for impurities moving across field lines.

The coefficients $\tau_z$, $\alpha_z$, $\beta_z$ are defined as

$$\tau_z = \frac{3(kT_i)^{3/2}m_Z^2}{4(2\pi m)^{1/2}e^4Z^2n_i\ln\Lambda(m + m_z)}$$

(2.15)

$$\alpha_z = 0.71Z^2$$

(2.16)

$$\beta_z = -3\frac{1 - \mu - 5\sqrt{2}Z^2(1.1\mu^{5/2} - 0.35\mu^{3/2})}{2.6 - 2\mu + 5.4\mu^2}$$

(2.17)

with $m$ being the mass of fuel ions, $\ln \Lambda$ the Coulomb logarithm and $\mu = m_v/(m_v + m)$ [33].

Out of the forces in equation 2.14, the ion and electron temperature gradient forces are directed towards the higher temperature in the upstream SOL region. The ion temperature gradient force tends to be several times stronger than the electron temperature gradient force; for example, in the case of W$^{10+}$ ions in a D$^+$ plasma and $T_e = T_i$, it is stronger by a factor of 3.7. The electrostatic force accelerates impurities towards the divertor targets, and is the most significant within the sheath and the magnetic pre-sheath. The friction force may act in either direction depending on the velocity of impurities relative to the fuel ions, although in the divertor its direction is generally towards the targets. The impurity pressure gradient force acts to diffuse impurities from higher towards lower impurity pressure.

The ability of the divertor and SOL plasma to deflect impurities from wall sources back towards the wall is called impurity screening. Screening consists of prompt redeposition, non-prompt local redeposition, and non-local redeposition of impurities which do not enter the main plasma. The most important factors in determining the screening efficiency are the ionisation mean-free path, the parallel-B impurity force balance, and potentially the radial and poloidal cross-field transport depending on the SOL conditions. The screening of heavy impurities is greatly enhanced by their tendency to ionise more readily than fuel ions (Fig. 2.4), placing most of the impurity ionisation source in a region of strong plasma flow towards surfaces. Geometrical effects, such as the solid angle of the main plasma at the erosion location, are significant when the ionisation mean-free path of impurities is larger or comparable to the size of the SOL. On
the other hand, the impact of divertor geometry on the screening of atomic impurities is negligible in dense high-recycling plasmas which ionise the impurities within millimetres of the surface.

2.2.4 Cross-field impurity transport mechanisms

Any force \( \vec{F} \) acting on a particle with charge \( q \), unless parallel to the magnetic field \( \vec{B} \), distorts the Larmor orbit of the particle and causes it to drift in the direction perpendicular to both the force and the magnetic field. The drift velocity is:

\[
\vec{v}_{\text{drift}} = \frac{\vec{F} \times \vec{B}}{qB^2}
\]  

(2.18)

Common examples of cross-field drifts in tokamak plasmas are the \( \vec{E} \times \vec{B} \) drift caused by the electric field and the grad-\( \vec{B} \) and curvature drifts caused by non-uniform \( \vec{B} \). The cross-field particle transport caused by Coulomb collisions is also a drift originating from perturbations in the electric and magnetic fields. In a fluid description of a plasma with pressure gradients, a diamagnetic \( \nabla p \times \vec{B} \) drift velocity also arises from the net motion of the fluid, although not related to the Larmor orbits of individual particles. Even gravity results in a drift, however the gravitational drift velocity tends to be negligible in comparison to other drifts.

The collisional kinetic theory of particle, momentum, and heat transport along and across magnetic field lines (equation 2.2), including the geometric effects and inhomogeneity of the fields, is known as neoclassical transport theory, to distinguish from earlier classical descriptions which neglected some or all effects of the magnetic geometry [34]. However, the cross-field transport observed in actual tokamak experiments is usually higher than implied from neoclassical transport [34], sometimes by 1–2 orders of magnitude. The contribution to the observed transport coefficients beyond neoclassical predictions is called anomalous. The total cross-field transport can thus be expressed as the sum of neoclassical and anomalous transport. The physics basis of anomalous transport is generally considered to be turbulent microinstabilities [35] and filamentary transport [36].

Both neoclassical and anomalous cross-field transport include diffusive and convective terms. Hence, the radial particle and heat fluxes can be written as:

\[
\Gamma_\perp = n(v_{nc} + v_{anom}) - (D_{nc} + D_{anom}) \frac{dn}{dr}
\]  

(2.19)

\[
q_\perp = 2kT\Gamma_\perp - (\chi_{nc} + \chi_{anom}) \frac{dT}{dr}
\]  

(2.20)

The neoclassical pinch velocity \( v_{nc} \) and the neoclassical diffusivity \( D_{nc} \) correspond to the drift vector (equation 2.4) and diffusion tensor (equation 2.5) respectively. More intuitively, a neoclassical inward pinch is

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Impurity erosion and transport processes in tokamaks created by the radial ion density gradient and a competing neoclassical outward pinch is created by the radial ion temperature gradient at low collisionality [37]. The neoclassical diffusive particle flux is proportional to the radial impurity density gradient. The total neoclassical particle flux can be summarised as [38]:

$$\Gamma_{nc} = -D_z \frac{\partial}{\partial r} \ln n_z + K_z \frac{\partial}{\partial r} \ln n_i + H_z \frac{\partial}{\partial r} \ln T_i \quad (2.21)$$

$D_z$, $K_z$, and $H_z$ are transport coefficients which depend nonlinearly on the collisionality of the plasma, impurity charge and mass, the geometry of the magnetic field and density profiles, and the fraction of trapped orbits. Trapped orbits are closed orbits which are poloidally confined to the low-field side by the magnetic field gradient. The ratio $H_z/K_z$ is called the temperature screening coefficient (TSC), a dimensionless quantity describing the direction of thermal convection and its relevance with respect to the inward convection driven by the ion density gradient. A negative TSC indicates outward thermal convection and a positive TSC indicates inward thermal convection. The TSC is interpreted as a measure of the effectiveness of the normalised ion temperature gradient $T_i^{-1} \partial T_i / \partial r$ relative to the normalised ion density gradient $n_i^{-1} \partial n_i / \partial r$ in offsetting the inward convection due to the density gradient. Temperature screening provides generally the highest outward convection at very low collisionality, but results in inward convection at high collisionality (Fig. 2.5). The strategy for achieving high fusion performance and mitigating W contamination in the planned ITER scenarios, and existing hybrid-scenario JET plasmas, depends to a large extent on efficient temperature screening of W in the pedestal region, predicted by neoclassical simulations and recently demonstrated in JET experiments [39].

Poloidal asymmetries in the impurity density, driven by parallel-B transport, also have a strong effect on neoclassical convection; impurities localised on the high-field side or the low-field side reduce or increase neoclassical convection respectively by 1–2 orders of magnitude, and may even reverse the direction of neoclassical transport [40]. The centrifugal effect due to toroidal rotation of the plasma is observed to outmatch other parallel-B dynamics on the closed flux surfaces in JET plasmas heated by neutral beam injection, causing heavy impurities to accumulate on the low-field side [41].

Calculating the anomalous transport coefficients from first principles requires appropriate computational tools and resources to resolve turbulence on the microscopic scale. Alternatively, in the case of experiments with available measurement data, the anomalous transport coefficients can be empirically inferred for interpretive modelling purposes, or predicted by empirical models which are validated against measurement data. In general, turbulent transport tends to be significant in JET at the pedestal.
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Figure 2.5. Neoclassical temperature screening coefficient of $W^{20+}$, $W^{40+}$, and $W^{60+}$ ions in a hypothetical plasma scenario as a function of collisionality. The calculation is based on analytical formulae [38] for the neoclassical transport coefficients $K_z$ and $H_z$, assuming a non-rotating plasma with a poloidally circular cross-section and a trapped particle fraction of 0.4.

...top and in the SOL [40], whereas neoclassical convection dominates JET heavy impurity transport near the magnetic axis and in the H-mode edge transport barrier [42].

In a steady state, the sum of neoclassical and anomalous convective particle fluxes must be compensated by opposite diffusive fluxes and particle sources. Assuming that the walls are both the source and the sink of impurities, an inward pinch velocity then creates a peaked radial impurity density profile in the main plasma. Conversely, an outward pinch velocity creates a hollow impurity density profile.

2.2.5 Impact of impurities on the fusion performance

Impurities affect the performance of a fusion plasma primarily through three mechanisms: dilution of fuel ions, energy losses due to electromagnetic radiation, and modified transport properties of particles and heat across flux surfaces. At a given electron density and ion temperature, dilution by a concentration $c_z = \frac{n_z}{n_e}$ of each impurity species $z$ with charge state $Z_z$ reduces the D-T fusion power $P_{fusion}$ according to the formula
Figure 2.6. The total radiative cooling factor of W calculated using three methods (AIM [44] (red), level-resolved (LR, black), and configuration-averaged (CA-LARGE, blue)) [45]. The contributions of bremsstrahlung (orange) and radiative and dielectronic recombination (grey) to the total W cooling factor are shown, as well as the fractional abundances of selected W ionisation stages.

\[
P_{\text{fusion}} = \int n_D n_T \sigma_{DT} (T_i) E_{DT} \, dV = \int \frac{1}{4} \left(1 - \sum_z c_z Z_z^2 \right)^2 n_e^2 \sigma_{DT} (T_i) E_{DT} \, dV
\]

(2.22)

Subscripts \(D\), \(T\), \(e\), \(i\), and \(z\) refer to deuterium, tritium, electrons, ions, and impurities respectively. \(\sigma_{DT}\) is the D-T fusion cross-section and \(E_{DT} = 17.6\) MeV is the energy released per fusion reaction.

The radiative energy losses due to impurities can be classified into bremsstrahlung and spectral line emission. The bremsstrahlung radiation \(\epsilon\) can be estimated as a function of wavelength \(\lambda\) as [43]:

\[
\epsilon(\lambda) = 0.95 \times 10^{-19} \frac{g_{ff} n_e^2 Z_{eff}^2 n_e T_e^{1/2}}{4 \pi \lambda} \exp \left(\frac{-h \lambda}{\lambda \gamma}\right) (\text{ph sr}^{-1} \text{m}^{-3} \text{nm}^{-1} \text{s}^{-1}).
\]

(2.23)

\(g_{ff} = 0.6183 \ln(T_e) - 0.0821\) is the electron free-free Gaunt factor, \(Z_{eff} = \sum_z n_z Z_z^2 n_e\) is the effective charge of the plasma, and \(h = 6.62607 \times 10^{-34}\) m\(^2\)kg/s is the Planck constant.

Spectral line emission of impurities occurs when bound electrons of impurity ions, atoms, or molecules transition from an excited energy state to a lower energy state. The excited electron states are created as a result of collisional excitation, recombination, or photoexcitation. The wavelength of the emitted radiation is unique to each electronic transition, which permits the inference of the impurity composition and charge state distribution from measured line emission spectra. The broadening, splitting,
Impurity erosion and transport processes in tokamaks and Doppler shifting of spectral lines, and the relative intensities of different lines, are also valuable methods of obtaining information about the plasma conditions such as density, temperature, and flow velocity. However, spectroscopic interpretation of heavy elements with more than 50 bound electrons is a massive computational challenge involving potentially billions of electronic transitions, which is why the typical uncertainty in the calculated photon emission coefficients for individual low-ionised high-Z spectral lines is up to an order of magnitude unless the coefficients can be validated against dedicated measurements. This is demonstrated by the comparison of the W cooling factor calculated using different methods (Fig. 2.6), which agree at fusion temperatures but deviate by a factor of 3 at typical SOL temperatures [45] due to simplifications necessitated by computational complexity.

Radiation losses in the core plasma undermine the energy confinement time and are thus undesirable when optimising for fusion performance. Line emission is the largest contribution to radiation losses caused by heavy impurities, such as tungsten, which retain several bound electrons even in the hottest region of the core plasma. Light impurities such as nitrogen and neon are fully ionised in the core plasma, which is why most of their radiation is emitted in the edge plasma instead.

W has a radiative cooling factor $> 10^{-31}$ Wm$^3$ at all electron temperatures up to the 10–20 keV expected in a D-T fusion reactor (Fig. 2.6). This implies that plasmas contaminated by W even at trace concentrations of order $10^{-4}$, although acceptable in terms of fuel dilution, are not viable for net energy production as they radiate significantly more energy than can be sustained by self-heating. The maximum realistically tolerable W concentration in a fusion plasma has been estimated as the range of several $10^{-5}$ [45].

Radiation in the divertor and main chamber SOL reduces the peak heat flux density at the strike points by distributing the heat more evenly across the vessel, thereby enabling the operation of higher-temperature plasmas within material heat tolerance limits and extending the duty cycle of wall components. Hence, reactor-relevant plasma scenarios tend to aim for the highest achievable fraction of radiated power to input heat flux within the edge and SOL. The deliberate injection of impurities into the plasma is called seeding, and it is a common method of increasing SOL radiation and reducing plasma temperature at the walls. The choice of seeding impurity species at a given radiated power is a compromise between fuel dilution, favouring elements with a higher cooling factor and thus more bound electrons, and core radiation losses, favouring the lighter elements with less electrons.

In contrast to the adverse effects of fuel dilution and core radiation losses, seeding of light and medium-Z impurities such as carbon, nitrogen, neon, and argon in moderate amounts is also observed to have a positive impact
Impurity erosion and transport processes in tokamaks on energy and particle confinement in the pedestal and core regions of many tokamaks [11, 46, 47, 48]. Physical mechanisms found by gyro-Landau fluid turbulence modelling to explain the improved pedestal confinement include enhanced $\vec{E} \times \vec{B}$ shearing due to stronger toroidal rotation gradients in the presence of impurities [11] as well as a stabilising effect of fuel dilution on the growth rate of turbulent instabilities called ion temperature gradient modes [48].

2.3 Impact of melting events and dust on the plasma

Plasma operations in tokamaks are subject to machine safety constraints, intended to protect the plasma-facing components and diagnostic instruments from excessive damage. Nevertheless, the heat tolerance limits of certain components were exceeded on rare occasions, due to unexpected plasma behaviour, operator error, or control system malfunction among other reasons. Due to such events, and due to intentional controlled melting studies, localised melting of wall components has been observed in several tokamaks [49]. Molten wall material may enter the plasma as droplets or contaminate the plasma via evaporation. Plasma-facing components deformed by melting were shown to compromise plasma performance, for instance completely preventing H-mode operation in a certain strike point geometry due to an accidentally created leading edge [50].

Loosely bound co-deposits on plasma-facing components may undergo flaking and become a source of dust inside the tokamak [51]. Dust is also created when small molten droplets or partially molten flakes of wall material re-solidify [51]. Dust has the potential to penetrate much further into the plasma than individual atoms before ionising, due to the innermost atoms of dust particles being shielded from interactions with the plasma. Thus, even if the divertor provides efficient screening of sputtered impurities, dust ejected from the divertor targets may severely contaminate the main plasma.

While melting and dust events have the potential to greatly increase the impurity content of the plasma, to the extent of terminating the plasma discharge, such events are uncommon and do not constitute a major impurity source compared to the total sputtering caused by the ordinary plasma discharges in JET [52]. In addition, secondary impurity sources created by one-off events decay over time and can be further mitigated by wall conditioning or maintenance [53]. Thus, in cases representing nominal plasma operations in present and future machines, thorough analysis of melting and dust events is not required for understanding plasma-wall interactions, impurity transport, and the impact of impurities on fusion performance.
3. Plasma diagnostics

Plasma diagnostics are scientific instruments which measure certain properties of the plasma. Diagnostics provide crucial data for interpreting plasma experiments, and for validating simulations and theoretical models. Real-time diagnostics also allow control systems to adjust the plasma parameters towards target values and to operate the device within safety limits.

3.1 Thomson scattering

Thomson scattering refers to the classical elastic scattering of electromagnetic radiation from free charged particles such as electrons. By observing the scattering of a laser beam due to its interaction with the plasma, the electron density and temperature can be inferred from the intensity of scattered light and the broadening of its spectral distribution along the laser line-of-sight. In JET, high-resolution Thomson scattering (HRTS) is applied to electron density and temperature measurements along the LFS mid-plane (Fig. 4.3).

3.2 Langmuir probes

A Langmuir probe is a diagnostic which measures the current-voltage characteristic of a plasma. Langmuir probe systems operate by applying bias voltages to electrodes inserted into the plasma and measuring the resulting electric current. At high negative or positive voltages with respect to the plasma, the current through the probe is nearly independent of the bias voltage, and known as the ion or electron saturation current, respectively. The voltage at which no current flows through the probe is referred to as the plasma floating potential. The electron temperature at the Debye sheath entrance can be inferred from the slope of the current-voltage curve in the region between the floating potential and the electron saturation
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current. The electron and ion density at the sheath entrance can then be calculated from the measured ion saturation current density by assuming that ions enter the sheath at the speed of sound $c_s = \sqrt{\frac{e(T_e + T_i)}{m_i}}$. The calculation of the ion sound speed depends on the inferred electron temperature, and on the typically unknown ion temperature, which is often assumed equal to the electron temperature in Langmuir probe analysis of tokamak plasmas.

3.3 Spectroscopy

3.3.1 Ultraviolet and visible spectroscopy

Most of the spectral line emission of atoms and low-charge ions in divertor plasmas is typically in the ultraviolet wavelength range. Additionally, many of the spectral lines valuable for divertor diagnostic purposes are in the visible spectrum. As the emitted wavelength is unique to each electronic transition, spectroscopy can be used to infer the density and charge state distribution of impurities if the electron density and temperature are known. Hence, ultraviolet and visible spectroscopy is one of the most versatile methods of diagnosing the SOL and divertor plasma conditions.

In this thesis, line-integrated measurements of the neutral hydrogenic emission line at 656 nm (Balmer-$\alpha$, more specifically D-$\alpha$ in the case of deuterium) and the singly ionised Be emission line at 527 nm (Be II) are used to validate the background plasmas, whereas neutral and singly ionised W emission lines (W I at 400.9 nm and W II at 364.0 nm, 434.8 nm respectively) are compared to synthetic diagnostics of the predicted W line emission to validate the predicted W erosion rate and transport of W$^{1+}$ ions.

3.3.2 Charge-exchange recombination spectroscopy

Charge-exchange recombination spectroscopy (CXRS) refers to measurements of the spectral line emission resulting from electrons recombining with ions in charge-exchange reactions. Like other forms of spectroscopy, CXRS provides information on the density and charge state distribution of impurities, although the analysis is applicable mostly to light impurities such as neon in the plasma edge, where charge-exchange reactions are frequent. CXRS also provides a measurement of the ion temperature through spectral line broadening.
3.3.3 Vacuum ultraviolet and soft X-ray spectroscopy

The wavelength range of 100–200 nm in the ultraviolet spectrum is strongly absorbed by the atmosphere and thus called vacuum-ultraviolet (VUV) radiation. VUV spectrometers often measure a wider range of wavelengths, extending into the extreme ultraviolet (XUV) range of 20–100 nm. VUV spectroscopy in this work refers to measurements using VUV spectrometers in the VUV and XUV ranges. W spectral line emission by charge states ranging from 2+ to 46+ has been identified in this wavelength range [54]. Soft X-rays (SXR) constitute the low-energy part of the X-ray spectrum below 5–10 eV, with lower penetration through materials compared to hard X-rays. The corresponding SXR wavelength range is approximately 0.2–20 nm. In hot plasmas, many W emission lines in the SXR range from different transitions and charge states merge into a quasi-continuum. The merging of W lines is particularly pronounced at 4–7 nm [55]. Due to the line merging, W line emission is difficult to distinguish from other sources of SXR emission in the same wavelength range. Individual spectral lines of highly charged \((W^{>50+})\) W emission in hot plasmas are more distinct in the sub-1 nm range [56].

3.4 Bolometry

Bolometry is the process of measuring the total radiated power incident on a surface by the means of temperature-dependent resistivity. When the relationship between bolometer temperature and its resistance, and the thermal conductance between the bolometer surface and a heat sink are known, the radiated power is inferred from the measured resistivity of the bolometer surface. Unlike spectroscopy, bolometry does not distinguish between electromagnetic radiation of different wavelengths, and can even be applied to particle radiation.

Using multiple collimated and intersecting bolometer lines-of-sight, the two-dimensional distribution of total radiated power in a cross-section of the plasma device can be tomographically reconstructed from the line-integrated measurements. In high-performance JET-ILW plasmas, the radiation emitted by the core plasma is dominated by W spectral line emission, enabling the cross-validation of VUV and SXR impurity measurements against bolometry and improving the spatial resolution of the measurements. The measurements of the W density in the JET main plasma studied in this thesis are based on integrated data analysis of cross-validated VUV, SXR, and bolometry, also taking into account the effects of light and medium-Z impurities as estimated from the measured effective charge of the plasma and from charge-exchange recombination spectroscopy [57].
3.5 Post-mortem tile analysis

Post-mortem tile analysis is the study of samples extracted from plasma-facing components after a series of plasma experiments. Post-mortem analysis is applied to estimate the net erosion and deposition rate and to determine the surface concentrations of different materials. Examples of post-mortem analysis techniques include nuclear reaction analysis, proton beam backscattering, and particle-induced X-ray emission [52]. In this thesis, results from post-mortem analysis are applied to justify the initial material composition of simulated JET divertor tiles (section 4.1.3) and to validate the predicted erosion and redeposition of marker samples in ASDEX Upgrade (section 5.3).
4. Simulating impurities in fusion plasmas

4.1 Edge plasma modelling tools

4.1.1 EDGE2D-EIRENE

EDGE2D-EIRENE is a computational code package consisting of the 2D multi-fluid edge plasma code EDGE2D [58] coupled to the Monte Carlo kinetic neutral transport code EIRENE [59]. EDGE2D solves the fluid equations (equations 2.11, 2.12, 2.13) in a discretised field-aligned representation of the tokamak 2D poloidal cross-section self-consistently for the electrons, main ions, and each impurity species. The simulation domain is divided into quadrilateral grid cells, organised by flux surface into poloidal rings and radially into rows. The grid is typically based on a magnetic equilibrium reconstruction of a real plasma discharge, but it is also possible to simulate hypothetical magnetic geometries. The EDGE2D-EIRENE simulations presented in this thesis are based on a single-null diverted plasma configuration, which entails a single X-point, two divertor targets, one SOL, one core region and one private flux region. The inner regions of the core plasma are replaced by a core boundary condition, as EDGE2D-EIRENE does not contain a predictive model for the deposition of auxiliary heating, neutral beam fuelling, or anomalous cross-field transport on closed flux surfaces.

The fluid equations in EDGE2D-EIRENE are most commonly solved in the parallel-B direction only, with cross-field transport treated as fully anomalous and diffusive with ad-hoc transport coefficients $D_\perp$, $\chi_{e,\perp}$, and $\chi_{i,\perp}$. However, EDGE2D-EIRENE is capable of including the cross-field drifts, albeit at a significantly increased computational cost and potentially unstable simulations. The fuel and impurity ion temperatures are assumed equal for numerical robustness and efficiency. CXRS measurements of the fuel and impurity ion temperatures in the DIII-D tokamak indicate
that the assumption of a single $T_i$ is justified in the core plasma, but not necessarily near the separatrix [60]. EDGE2D-EIRENE has an adaptive time step, allowing it to resolve the time evolution of rapidly changing conditions such as the onset and decay of ELMs or the plasma response to updated input settings, without compromising computational efficiency when approaching a steady state.

The boundary conditions for ion and impurity density are determined by particle flux and parallel-B velocity at the divertor targets, by an exponential density decay length at the radial outer boundaries of the SOL and the PFR, and by an imposed fuelling rate at the core boundary. The parallel-B momentum boundary condition is set by either a sonic (M=1) or supersonic (M>=1) flow velocity at the sheath entrance, and an imposed flow velocity at the core boundary. The electron and ion heat flux boundary conditions are given as heat transmission coefficients across the sheath, an imposed temperature decrease across the radially outermost rings, and an imposed ion and electron heat flux across the core boundary.

The EDGE2D plasma solution is provided as input to EIRENE for a calculation of atomic and molecular reaction rates as well as plasma-surface interactions (section 2.1). EIRENE returns the recycled, reflected, and eroded particle and heat fluxes from wall surfaces, the atomic and molecular densities, the power and momentum sources and sinks due to plasma-neutral reactions, and the volumetric ionisation and recombination densities between the neutral and singly ionised state. Perpendicular incidence is assumed for the fluid ions. The EIRENE output is used as source and sink terms in the EDGE2D fluid equations for the next time steps until EIRENE is called again with an updated plasma solution.

EDGE2D-EIRENE includes an ad-hoc model of simulating ELMs. During an ELM, the anomalous pinch velocity and the particle and heat cross-field diffusivities are multiplied by specified transport multipliers within a specified ELM-affected region. The EDGE2D-EIRENE simulations in this thesis assume zero pinch velocity and an ELM-affected region consisting of the pedestal and near-SOL regions on the low-field side of the main chamber. Other plasma regions are affected by the ELMs indirectly, due to changes in the plasma conditions, but they do not have increased cross-field diffusivities during an ELM.

The times at which ELMs are triggered, the duration of the ELMs, the values of the transport multipliers, and the boundaries of the ELM-affected region are all free input parameters. Thus, the EDGE2D-EIRENE ELM model is of limited predictive value, but a versatile interpretive model when fitted to measurement data. EDGE2D-EIRENE also includes kinetic correction factors [61] for the heat flux limiters and the sheath heat transmission factors.

The many charge states of heavy impurities such as W are bundled into a lower number of fluid species for computational efficiency and numerical
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robustness. The reference bundling scheme for W in this thesis includes 6 fluid species representing W charge states 1+, 2+ to 6+, 7+ to 12+, 13+ to 22+, 23+ to 73+, and fully ionised 74+. Each fluid species is assigned a locally varying non-integer average charge state based on the ionisation and recombination balance and the transport to and from adjacent grid cells.

When a non-recycling impurity is deposited on a surface, the surface material composition remains unchanged as EDGE2D-EIRENE does not model material mixing or re-erosion. To address this shortcoming in this thesis, the re-erosion of Be from W surfaces is emulated in EDGE2D-EIRENE by artificial atomic Be injection at the divertor targets. The imposed Be sources are radially uniform, and their size and location are chosen such that the sources cover the locations of peak incident D ion flux. Here, the Be injection rate is adjusted to reproduce the measured spectral line emission of the Be II line at 527 nm, ensuring a more realistic Be concentration in the divertor plasma than if re-erosion was neglected.

4.1.2 DIVIMP, OEDGE

DIVIMP [62, 63] is a 2D trace-impurity Monte Carlo code based on the parallel-B impurity force balance model (equation 2.14) to calculate the acceleration of individual test particles in a fluid background plasma. The Larmor orbits of ions are not modelled. Cross-field transport is treated as anomalous with ad-hoc transport coefficients, with the optional inclusion of the $\vec{E} \times \vec{B}$ drifts.

Compared to EDGE2D-EIRENE, DIVIMP has two major advantages: short execution time and the ability to resolve every impurity ionisation state without numerical complications. The main drawbacks of DIVIMP are the lack of impurity effects on the imported background plasma conditions and the partially incomplete implementation of cross-field transport, e.g. lack of grad-$\vec{B}$ drifts.

DIVIMP is part of a code package called OEDGE, which also consists of a background plasma solver based on the onion-skin model (OSM) and EIRENE for neutral transport. OSM is a method of calculating the plasma conditions from imposed divertor target conditions towards the upstream, individually for each flux surface. OSM is a computationally inexpensive way of obtaining a background plasma solution, but requires prior knowledge of the target conditions and is based on a less comprehensive physics model than multi-fluid codes such as EDGE2D-EIRENE.

In this thesis, all DIVIMP simulations are based on an EDGE2D-EIRENE background plasma solution and a W ionisation source imported from EDGE2D-EIRENE. The DIVIMP simulation domain is the same as in the EDGE2D-EIRENE simulations. DIVIMP contains the option to independently predict impurity erosion as well as an analytical model for estimat-
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ing prompt redeposition, however these were replaced by the EDGE2D-EIRENE \( W^{1+} \) ion source to achieve an unbiased comparison of the ion transport models of the two codes. The input parameters and boundary conditions are chosen as close to the EDGE2D-EIRENE setup as possible. Further details of the applied DIVIMP options are explained in publications I and II.

### 4.1.3 ERO and ERO2.0

ERO \[64\] and ERO2.0 \[65\] are 3D full-orbit kinetic trace-impurity Monte Carlo codes for simulating impurity erosion, transport and redeposition in plasma devices. The ion transport model of both codes is based on the Fokker-Planck equation (equation 2.2). ERO is limited to a cuboid simulation volume covering a selected region of interest, whereas ERO2.0 is capable of simulating the entire plasma volume and all of the plasma-facing components. ERO2.0 is also compatible with scalable parallelised computing and contains a large amount of performance optimisations compared to ERO.

Compared to EDGE2D-EIRENE and DIVIMP, ERO and ERO2.0 have a significantly more sophisticated model of plasma-surface interactions, including the dependence of the sputtering yield on the impact angle, a kinetic treatment of prompt redeposition, and the ability to track material mixing and re-erosion of deposited material. The ion transport model is fully kinetic, requiring fewer approximations than EDGE2D-EIRENE and DIVIMP, and with cross-field drifts intrinsically included without the major detrimental impact on code performance or stability. ERO2.0 also includes a 3D geometry with toroidally non-uniform plasma-facing components. ERO2.0 is capable of simulating impurity transport in toroidally asymmetric background plasmas as well, however in this thesis the background plasmas are imported from EDGE2D-EIRENE and toroidal symmetry is assumed. Unlike EDGE2D-EIRENE, ERO and ERO2.0 do not model impurity effects on the background plasma. Compared to DIVIMP, some ERO2.0 simulations require 2–3 orders of magnitude more computational time despite parallelisation to 16–24 CPUs.

The ERO2.0 calculations of the W erosion rate presented in this thesis are based on JET divertor plasma-facing components with a mixed material composition of Be and W (Fig. 4.1). The assumed surface concentrations of Be and W are based on a combination of post-mortem tile analysis \[52\] and earlier ERO2.0 modelling of Be and W mixing in the JET divertor \[66\]. The limiters in the main chamber are assumed to be 100% Be. The Inconel vacuum vessel and other main chamber structures beyond the limiters are not modelled, but instead a fully absorbing toroidally symmetric boundary is placed at the radially outermost extent of the limiter surfaces.

The centrifugal effect due to the rotation of the plasma was newly im-
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implemented in ERO2.0 as part of this thesis project. The centrifugal effect creates a pseudo-force due to the rotating frame of reference, accelerating ions towards larger major radius. The effect is particularly important for predicting the poloidal asymmetries of heavy impurities in the main plasma. The first ERO2.0 predictions of such asymmetries are presented in this thesis.

![Image of divertor tiles in JET](image1.png)

**Figure 4.1.** a) Labeling of the divertor tiles in JET. b) Initial Be and W surface concentration of JET divertor tiles assumed in the ERO2.0 simulations.

The background plasma solutions produced by EDGE2D-EIRENE consist of a 2D poloidal representation of the magnetic field, the electron density, the ion and electron temperatures, the parallel-B ion flow velocity, the parallel-B and radial electric field components, and the ion and electron conductive parallel-B heat fluxes. The quantities are interpolated from the EDGE2D-EIRENE field-aligned quadrilateral grid onto a higher-resolution 2D Cartesian grid and converted into three dimensions assuming toroidal symmetry. Outside the EDGE2D-EIRENE computational domain, nearest-neighbour extrapolation is applied in the core plasma region and an exponential decay is assumed for radial extrapolation between the EDGE2D-EIRENE domain boundary and the plasma-facing components.

The radial electric field, which is missing from the EDGE2D-EIRENE output when cross-field drifts are disabled, is calculated based on the elec-
tron temperature profile using the approximation $E_{\text{rad}} = -3/e \frac{dT_e}{dr}$ [67] on open flux surfaces. On closed flux surfaces, the radial electric field is assumed to be zero.

The atomic fluxes incident on each wall location are extracted from EIRENE simulations to calculate the sputtering rates due to atom impact in ERO2.0. The temperature of the incident atoms is based on the average impact energy predicted by EIRENE for Be wall components. However, for W components, converting the atomic energy spectrum directly into a single temperature would severely underestimate the erosion, because the average energy is significantly lower than the sputtering threshold and W erosion by D atoms is caused by a non-Maxwellian high-energy tail. To alleviate the bias due to assuming a Maxwellian distribution for the incident atoms, the atomic fluxes and temperatures onto W components are adjusted in pre-processing by discarding atoms with energy below 200 eV. Thus, the flux and temperature passed as input to ERO2.0 represent only the high-energy tail of the atomic distribution which contributes to W erosion.

The ERO2.0 sputtering and reflection yields are based on SDTrimSP6 [68] data, with fallback to SDTrimSP5 [69] data in case of material combinations for which SDTrimSP6 calculations do not exist in the repository. The SDTrimSP versions are based on the same physics except for a number of model extensions and new options in SDTrimSP6 which are unlikely to have a major impact on the results in this thesis. The impact angle of background ions and atoms is assumed to be 60° with respect to the surface normal. Contrary to the initial ERO2.0 implementation of fluid-like thermal forces, a revised kinetic treatment of the thermal forces [70] is applied. The anomalous cross-field diffusivity is assumed to be a constant 1 m²/s and the anomalous cross-field convective velocity zero. A constant timestep of $10^{-8}$ seconds is used. Chemical erosion and sputtering due to molecules is not modelled.

### 4.2 Core plasma modelling tools

#### 4.2.1 JETTO and SANCO

JETTO [71] is a fluid code for modelling cross-field ion and electron transport in the core plasma. JETTO operates on a one-dimensional geometry, only calculating radial profiles, although some higher-dimensional effects are also taken into account in the calculation of the transport coefficients. In fully predictive simulations, JETTO solves conservation equations for plasma current, electron and ion temperature, ion density, and toroidal momentum. JETTO can also be executed with one or more of the equa-
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JETTO incorporates a multitude of computational tools and models to enable more advanced and realistic simulations. SANCO is the impurity transport modelling tool within JETTO, compatible with a variety of neoclassical and anomalous transport models. PENCIL is a tool which calculates the electron and ion heat deposition profiles and torque due to neutral beam injection. FRANTIC and EIRENE are tools for atomic and molecular transport; FRANTIC is a computationally efficient and simple ad-hoc fluid description of atoms only, whereas EIRENE is a more sophisticated but computationally more demanding kinetic Monte Carlo treatment of atoms and molecules. NCLASS [72] is a one-dimensional transport model which computes the neoclassical diffusivities and convective velocities.

Like EDGE2D-EIRENE, JETTO also includes ad-hoc treatments of the edge transport barrier and ELMs. Due to the one-dimensional geometry of JETTO, the ELM-affected region is poloidally symmetric rather than localised near the low-field side mid-plane. Both codes have transport multipliers applied to ions, electrons, and heat starting at the prescribed ELM start times and lasting for a prescribed duration. In JETTO, the ELM transport multipliers are applied with a Gaussian-shaped weighting centered at a prescribed radial location, as opposed to prescribed inner and outer radial boundaries for the ELM-affected region like in EDGE2D-EIRENE.

JETTO includes a transport code interface, which allows the user to select the anomalous and neoclassical transport models from a selection of empirical (e.g. Bohm-gyro-Bohm, section 4.2.2) and first-principle transport codes (e.g. QuaLiKiz, section 4.2.3 and NEO, section 4.2.4). When selected, the transport model is applied to both main ion transport in JETTO and impurity transport in SANCO. It is also possible to use NCLASS for main ion neoclassical transport and NEO for impurities only.

EDGE2D-EIRENE together with JETTO, SANCO, and the other modelling tools coupled to them constitute the JINTRAC suite of codes for integrated modelling [73, 74].

4.2.2 Bohm-gyro-Bohm transport

The Bohm-gyro-Bohm (BgB) transport model [75] is an empirical model for anomalous heat and particle transport, in which the total diffusivity is the sum of two terms called the Bohm and gyro-Bohm components. The Bohm term, inversely proportional to the magnetic field $B_t$, is dominant in the plasma edge, whereas the gyro-Bohm term proportional to $B_t^{-2}$ is more significant in the center of the plasma. Both terms are multiplied by ad-hoc scaling constants determined by fitting the model to a database of...
plasma discharges from JET and other tokamaks.

While BgB tends to yield fast and relatively accurate predictions in conditions similar to the discharges in its fitting database, there is less confidence that the model can be extrapolated to future machines compared to models derived from first principles. An advantage of using BgB in JETTO for interpretive background plasma simulations is that the simulation can be rapidly iterated multiple times with adjusted transport scaling factors to find close agreement with measurement data.

4.2.3 QuaLiKiz

QuaLiKiz (QLK) [76, 77] is a 3D quasilinear gyrokinetic transport code for modelling turbulent transport due to microinstabilities. Integrated into JINTRAC, QLK calculates the anomalous cross-field diffusivities and convective velocities for electrons, each ion species, angular momentum, and heat. The transport coefficients are used to calculate the time evolution of 1D radial plasma profiles, although the calculation of the coefficients includes also higher-dimensional effects.

QLK simulations tend to require up to several million times more computational resources than JETTO simulations with BgB transport. To enable turbulence simulations in a more practical timeframe, databases of QLK simulations covering multidimensional parameter scans were compiled and used to train neural networks to predict fast approximate QLK solutions [78]. A 10-dimensional neural network [78] and more recently a 15-dimensional neural network [79] cover a selected subset of the parameter space, approximating QLK solutions for several orders of magnitude lower computational cost compared to actual, non-surrogate QLK simulations without a neural network.

4.2.4 NEO

NEO [80] is a neoclassical core plasma transport code which includes a drift-kinetic treatment of the Fokker-Planck equation (equation 2.2) with a linearised collision operator. NEO accounts for poloidal asymmetries and the impact of toroidal rotation on neoclassical convection, which is why NEO is a far more appropriate tool for modelling heavy impurity transport compared to 1D neoclassical transport models such as NCLASS. When applied to JETTO/SANCO simulations, the poloidally asymmetric transport calculated by NEO is converted into one-dimensional effective cross-field transport coefficients for compatibility with the 1D geometry of JETTO, but the higher-dimensional solutions are also stored in a separate output file to allow the reconstruction of the 2D poloidally asymmetric density profiles.

The NEO transport model is based on the traditional neoclassical order-
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which asserts that the ion Larmor radius is much smaller than the length scale of gradients in the plasma conditions. This is a valid assumption for most of the confined plasma, except it is potentially violated within the edge transport barrier of H-mode discharges. To mitigate the issue of an invalid transport model, in this thesis NEO is applied to W transport only in the region inside the pedestal top. The flux-surface averaged W density at the pedestal top predicted by ERO2.0 W erosion and edge plasma transport modelling is matched in NEO by adjusting the W boundary condition at the separatrix.

4.3 Modelling workflow and simulated plasma scenarios

![Figure 4.2. Workflow of each background plasma and impurity modelling approach presented in this thesis.](image)

The modelling process and use of computational tools in this thesis is illustrated in Fig. 4.2. JINTRAC, EDGE2D-EIRENE, DIVIMP, and ERO2.0 are applied to JET discharges (Publications I-III), whereas OEDGE and ERO are applied to ASDEX Upgrade discharges (Publication IV). An overview of the modelled discharges is presented in Table 4.1. In Table 4.1, V5/C means vertical high-field side target / tile 5/C low-field side target strike point configuration (Fig. 4.3), C-C means the strike points are in the divertor corners (Fig. 4.4), and V-V refers to vertical high- and low-field side strike points (Fig. 4.5c).

In this thesis project, the chosen modelling approaches progressed from the less complex and more comprehensively characterised L-mode plasmas
Table 4.1. Overview of JET and ASDEX Upgrade plasma discharges modelled and discussed in this thesis. $P_{aux}$ and $P_{Ohmic}$ are respectively the auxiliary and resistive heating power. All the listed discharges except JPNs 98914 and 99151 have deuterium as the main ion species.

<table>
<thead>
<tr>
<th>Discharge</th>
<th>Time</th>
<th>$B_t$</th>
<th>$I_p$</th>
<th>$P_{aux}$</th>
<th>$P_{Ohmic}$</th>
<th>Targets</th>
<th>$n_{e,sep,OMP}$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>JPN 81472</td>
<td>9 s</td>
<td>2.5 T</td>
<td>2.5 MA</td>
<td>1 MW</td>
<td>1.5 MW</td>
<td>V5/C</td>
<td>$0.8\cdot10^{19}$ m$^{-3}$</td>
<td>L-mode</td>
</tr>
<tr>
<td>JPN 82486</td>
<td>14 s</td>
<td>2.0 T</td>
<td>2.0 MA</td>
<td>10 MW</td>
<td>1 MW</td>
<td>V5/C</td>
<td>$2.8\cdot10^{19}$ m$^{-3}$</td>
<td>ELMy H-mode</td>
</tr>
<tr>
<td>JPN 83393</td>
<td>21 s</td>
<td>2.0 T</td>
<td>2.0 MA</td>
<td>6 MW</td>
<td>1 MW</td>
<td>V5/C</td>
<td>$3.5\cdot10^{19}$ m$^{-3}$</td>
<td>Inter-ELM H-mode</td>
</tr>
<tr>
<td>JPN 94605–07</td>
<td>10 s</td>
<td>2.5 T</td>
<td>2.3 MA</td>
<td>18 MW</td>
<td>1 MW</td>
<td>V5/C</td>
<td>$3.2\cdot10^{19}$ m$^{-3}$</td>
<td>ELMy H-mode</td>
</tr>
<tr>
<td>JPN 94606</td>
<td>15 s</td>
<td>2.5 T</td>
<td>2.3 MA</td>
<td>18 MW</td>
<td>1 MW</td>
<td>C-C</td>
<td>$2.4\cdot10^{19}$ m$^{-3}$</td>
<td>JPN 94605 with C-C</td>
</tr>
<tr>
<td>JPN 96947</td>
<td>8 s</td>
<td>3.4 T</td>
<td>2.3 MA</td>
<td>35 MW</td>
<td>0.5 MW</td>
<td>C-C</td>
<td>$1.8\cdot10^{19}$ m$^{-3}$</td>
<td>Hybrid ELMy H-mode</td>
</tr>
<tr>
<td>JPN 97781</td>
<td>8 s</td>
<td>3.4 T</td>
<td>2.3 MA</td>
<td>32 MW</td>
<td>0.5 MW</td>
<td>C-C</td>
<td>$2.0\cdot10^{19}$ m$^{-3}$</td>
<td>Hybrid ELMy H-mode</td>
</tr>
<tr>
<td>JPN 98914</td>
<td>9 s</td>
<td>2.5 T</td>
<td>2.3 MA</td>
<td>20 MW</td>
<td>1 MW</td>
<td>V5/C</td>
<td>$3.2\cdot10^{19}$ m$^{-3}$</td>
<td>JPN 94605 with T</td>
</tr>
<tr>
<td>JPN 99151</td>
<td>8 s</td>
<td>3.4 T</td>
<td>2.3 MA</td>
<td>31 MW</td>
<td>0.5 MW</td>
<td>C-C</td>
<td>$2.2\cdot10^{19}$ m$^{-3}$</td>
<td>Hybrid with T</td>
</tr>
<tr>
<td>AUG 35609–17</td>
<td>-</td>
<td>2.5 T</td>
<td>0.8 MA</td>
<td>0.7 MW</td>
<td>0.3 MW</td>
<td>V-V</td>
<td>$0.7\cdot10^{19}$ m$^{-3}$</td>
<td>L-mode</td>
</tr>
</tbody>
</table>

The EDGE2D-EIRENE background plasmas representing JET experiments are validated against Thomson scattering measurements of $n_e$ and $T_e$ along the LFS mid-plane, and to Langmuir probe measurements of $n_e$, $T_e$, and $j_{sat}$ along the LFS divertor target in cases where such measurements are available. The EDGE2D-EIRENE plasma scenarios modelled for Publications II-III (JPNs 81472, 82486, 94605–94607, 96947, 98914, 99151) include Be injection at both divertor targets emulating the re-erosion of Be, validated against spectroscopic measurements of the Be II line emission at 527 nm. Background plasmas of experiments with available upstream ion temperature measurements based on charge-exchange recombination spectroscopy are also validated against the upstream ion temperature. Additionally, to more accurately constrain the assumed ELM and edge
to inter-ELM H-mode, then ultimately time-dependent type-I ELMy H-mode simulations including several ELM cycles. The modelled L-mode scenarios focus on the low-recycling regime, because the background plasma simulations yield the most robust and accurate predictions at low-recycling conditions, and because W erosion is less prevalent and more challenging to accurately diagnose in the high-recycling and detached regimes. V5/C is the reference divertor configuration in all of the JET-related publications (I-III) due to its optimal diagnostic coverage, whereas the target conditions in the simulated C-C discharges are largely predictive. The predictive uncertainty of the C-C target conditions is significantly alleviated by the high heating power (>18 MW) and relatively low density in the SOL ($n_u < 2.5\cdot10^{19}$ m$^{-3}$ in H-mode), resulting in nearly isothermal low-recycling SOL conditions in the modelled discharges.

The EDGE2D-EIRENE background plasmas representing JET experiments are validated against Thomson scattering measurements of $n_e$ and $T_e$ along the LFS mid-plane, and to Langmuir probe measurements of $n_e$, $T_e$, and $j_{sat}$ along the LFS divertor target in cases where such measurements are available. The EDGE2D-EIRENE plasma scenarios modelled for Publications II-III (JPNs 81472, 82486, 94605–94607, 96947, 98914, 99151) include Be injection at both divertor targets emulating the re-erosion of Be, validated against spectroscopic measurements of the Be II line emission at 527 nm. Background plasmas of experiments with available upstream ion temperature measurements based on charge-exchange recombination spectroscopy are also validated against the upstream ion temperature. Additionally, to more accurately constrain the assumed ELM and edge
transport barrier parameter values, the type-I ELMy H-mode discharges with $P_{aux}=18$ MW or greater are validated against the ELM-resolved time-evolution of the pedestal electron temperature and density, the plasma stored energy, and the heat loads on divertor targets, as measured by conditionally averaged Thomson scattering, fast magnetic equilibrium reconstruction, and divertor infrared cameras respectively. Figures demonstrating the validation steps of matching the background plasma conditions to experimental measurements are included in Appendix A.

To characterise the short-range migration of eroded impurities experimentally and computationally, a series of dedicated ASDEX Upgrade L-mode experiments was analysed and modelled, as equivalent data is not available for JET. The ASDEX Upgrade discharges #35609–35617 studied the erosion and redeposition of gold (Au) marker samples (section 5.3) of sizes 1x1 mm and 5x5 mm applied on a molybdenum (Mo) coating layer (Fig. 4.5a). The boundary conditions for OEDGE modelling of the background plasma were obtained from Langmuir probe measurements along the LFS divertor target. To quantify the uncertainties of the background plasma modelling, three background plasma scenarios referred to as low-n (reduced electron density by a factor of 3), BC (base case), and high-T (electron temperature increased from 25 to 40 eV at the LFS strike point) were compared. The impurity concentrations of boron ($c_B$), carbon ($c_C$), nitrogen ($c_N$), and tungsten ($c_W$) were varied from $c_B=c_C=0.005$, $c_N=0.0075$, $c_W=5 \times 10^{-5}$ to $c_B=c_C=0.0075$, $c_N=0.01$, $c_W=1 \times 10^{-4}$, corresponding to effective charges $Z_{\text{eff}}$ of 1.93 and 2.47, respectively. In addition, a set of ERO simulations studying the erosion of hypothetical W markers instead of Au was conducted with initial $c_W=0$ in the plasma, resulting in $Z_{\text{eff}}=1.66$. A comparison of the resulting OEDGE background plasmas to Langmuir probe data is included in Appendix A.
Simulating impurities in fusion plasmas

Figure 4.3. Magnetic geometry of JPN 81472 at 9 s and JPN 83393 at 21 s in the vertical tile 3 - horizontal tile 5/C (V5/C) target configuration, illustrated in a poloidal cross-section of JET together with the high-resolution Thomson scattering (HRTS), lithium beam (Li-beam), reciprocating upstream Langmuir probe (RCP), and low-field side divertor target Langmuir probe (LPs) diagnostics used for validation of the EDGE2D-EIRENE background plasma conditions.
Figure 4.4. Corner-corner divertor target configuration of JET discharges JPN 94606 at 15 s (red) and JPN 96947 at 8 s (blue).
Figure 4.5. a) Photographs of the marker samples before and after plasma exposure in ASDEX Upgrade experiments. b) Experimentally measured net erosion (negative) and deposition (positive) rates of the Au markers and the Mo coating of the samples. The grey area illustrates typical uncertainty in the separatrix location. c) The vertical-vertical divertor target configuration of the studied ASDEX Upgrade plasma discharges and the simulation volume of ERO.
5. Prediction and validation of heavy impurity erosion and transport

This chapter presents the main results of Publications I-IV, as well as results which are relevant to the research topics of the thesis, but are yet to be published as a journal article.

The primary reasons for differences in W transport predictions between DIVIMP and EDGE2D-EIRENE are discussed, and the impact of the predicted W charge state on W transport in the SOL is explained (section 5.1, publication I).

The predicted W erosion in JET L-mode and H-mode plasmas, the contributions of each incident particle species to W sputtering, and the dependence of the W erosion rate on the plasma parameters is described (section 5.2, publications II and III). The validation is focused on the LFS divertor target due to its more comprehensive diagnostic coverage, and due to the higher accuracy of background plasma simulations in reproducing the measured plasma conditions compared to the HFS target.

The simulated and observed net and gross erosion and deposition of Mo and Au marker samples is analysed in ASDEX Upgrade L-mode experiments (section 5.3, publication IV). The study characterises the short-range migration of sputtered impurities. The feasibility of using Au markers in lieu of W for erosion studies in W devices is demonstrated.

The divertor screening of W at different locations in JET, predicted by DIVIMP and EDGE2D-EIRENE, is compared by varying the location of a simulated W source of constant magnitude (section 5.4).

The main plasma W density in JET L-mode and type-I ELMy H-mode plasmas predicted by JINTRAC is validated against the experimentally inferred W density profiles (section 5.5, publication II). In addition to the integrated core-edge JINTRAC simulations of publication II, more recent predictions using ERO2.0 for W erosion and edge transport and JINTRAC with NEO for neoclassical core transport are presented and validated.
Figure 5.1. Average charge state of W ions in JET L-mode discharge #81472 as a function of the local electron temperature predicted by DIVIMP and EDGE2D-EIRENE with a) EDGE2D-EIRENE bundling W to 6 fluid species and b) with each charge state up to 20+ treated as a separate fluid species. Each marker represents one grid cell in the discretised computational domain. The same ADAS ionisation and recombination rates are used by both EDGE2D-EIRENE and DIVIMP. Figure based on Publication I.
5.1 Impact of the bundling of charge states on W average charge

EDGE2D-EIRENE simulations with W ion charge states bundled into 6 fluid species predict up to 40% lower average W charge in the SOL of a JET L-mode plasma, compared to DIVIMP simulations without any bundling of charge states (Fig. 5.1a). EDGE2D-EIRENE simulations with a separate fluid species for every W charge state from 1+ to 20+ closely reproduce the distribution of W charge states predicted by DIVIMP, demonstrating that the reduction in the predicted average W charge is due to charge state bundling and not due to other differences between the simulation tools (Fig. 5.1b). The bundling does not significantly affect the average W charge in far-SOL regions with $T_e < 10$ eV, or on closed flux surfaces with $T_e > 150$ eV on which W reaches an ionisation equilibrium. The study of W bundling effects was repeated in an inter-ELM H-mode JET plasma with similar results (Publication I, Fig. 6).

DIVIMP and less bundled EDGE2D-EIRENE simulations (Fig. 5.1b) indicate that the average charge of W in different regions of the SOL depends not only on the local electron temperature, but also strongly on the predicted flows of W in and out of the confined plasma and into the divertor. W ions which have obtained a typical charge of 13+ to 18+ in the edge of the confined plasma (100 eV < $T_e$ < 200 eV) are unlikely to recombine much below 13+ when they reenter the SOL until they are redeposited, because the timescale of parallel-B transport into the divertor is much shorter than the time required for high W charge states to recombine back into ionisation equilibrium in the SOL. W ions which did not enter the main plasma remain at significantly lower charge states than W ions exiting the main plasma. This explains the bifurcated distribution of average W charges at electron temperatures between 10 and 100 eV (Fig. 5.1b). The bundling of W charge states 2+ to 6+ and 7+ to 13+ into shared fluid species leads to a severe underprediction of the W charge bifurcation and incorrectly suggests that the local electron temperature is the single most important factor in determining the average W charge.

5.1.1 Implications of charge state bundling for W transport

Underpredicted average W charge states in the SOL lead to reduced W density in the main chamber near-SOL and in the main plasma. The reason for the reduction in W density is that the primary parallel-B forces acting on W, the thermal and friction forces, are proportional to the square of the charge state, whereas the inertia of W ions is virtually independent of their charge. Hence, the parallel-B confinement of highly charged W ions in the main chamber near-SOL is far more effective than that of low-charge W ions. At a given ion temperature, highly-charged W ions are on average confined in the SOL for a longer time than lower-charged ions,
and therefore the same W source results in a higher W density when the average W charge is higher.

Previous investigations [82] of W charge state bundling effects found that EDGE2D-EIRENE predicts the total W density to be nearly independent of the W bundling scheme, with density variations no greater than 25% between fully resolved and single-fluid bundled treatment of W charges in the SOL. The findings contradict the expected reduction in W density due to lower average W charge based on Fig. 5.1a, as well as the observed consistent 50% difference between total W concentration predicted by DIVIMP and EDGE2D-EIRENE (Fig. 5.17). The contradiction is explained by the fact that highly-resolved W bundling schemes violate the conservation of momentum in EDGE2D-EIRENE due to numerical complications. Despite a more accurate distribution of W charge states and more detailed calculations of the W parallel-B force balance, EDGE2D-EIRENE produces unphysical output such as spatially constant flow velocities for certain W charge states when the W ions are separated into many low-density W fluid species. Thus, the least unphysical EDGE2D-EIRENE predictions of W density are obtained by bundling the W charge states, despite the systematic bias induced by the incorrectly predicted average W charge.

In addition to reducing the main plasma W density, the underpredicted W charge states also change the predicted deposition pattern of W in the divertor. When the W charge is lower and the near-SOL accumulation of W is weaker, there is more parallel-B transport of W from the main chamber into the divertor near the strike points. Conversely, when the higher-charged W ions are trapped along field lines in the main chamber near-SOL, they must travel radially further outwards before they are able to reach the divertor, resulting in reduced W deposition in the near-SOL and increased W deposition in the far-SOL divertor.

The W density in the main plasma is determined by the balance of cross-field W transport to and from the separatrix, which means that the W density profile across the entire confined plasma is linearly proportional to the W density at the separatrix. For example, if the underestimation of the average W charge leads to a 50% discrepancy between bundled and unbundled W density at the separatrix, that same 50% discrepancy propagates into all of the confined plasma. To avoid accumulating uncertainty, W charge states should not be bundled unless necessary for computational reasons. On the other hand, quantitative knowledge of the effects of charge state bundling makes it possible to compensate for the reduced W density when unbundled W simulations are not available. Based on the comparison between DIVIMP and EDGE2D-EIRENE predictions, the main plasma W density predicted by EDGE2D-EIRENE should be multiplied by a factor of 1.5 to compensate for the effects of W bundling.
Prediction and validation of heavy impurity erosion and transport

5.2 W erosion in the JET divertor

5.2.1 W erosion in JET L-mode

EDGE2D-EIRENE predicts that Be is the largest contributor to gross W erosion in JET-ILW attached L-mode plasmas (Fig. 5.2), consistent with analysis based on spectroscopic measurements [17]. At the highest electron temperatures of >50 eV in the divertor, there are also significant contributions of W erosion due to D+ and W self-sputtering. In regions of low electron density, the dominant cause of W sputtering is energetic D atoms created by charge-exchange reactions primarily from the edge of the confined plasma. Be atoms reflected from the targets add a minor contribution of <10% to the W sputtering rate, mostly at lower densities.

As the D fuelling rate, and consequently also the upstream electron density, is increased from low-recycling towards high-recycling and detached divertor conditions, the W sputtering rates due to each particle species decrease disparately (Fig. 5.2). The contribution of D+ ions to W sputtering becomes negligible as the divertor electron temperature decreases below 50 eV, reflected Be atoms are negligible below 40 eV, W self-sputtering below 35 eV, and Be ions below 15 eV. W sputtering by charge-exchange D atoms is the process least sensitive to the SOL conditions, and the only significant source of W in detached plasmas. Nonetheless, even the W source due to D atoms is 2–3 orders of magnitude weaker in detached plasmas than in the low-recycling regime. The total W sputtering rate is approximately an exponentially decreasing function of the upstream electron density $n_{e,sep}$, reduced by half every time $n_{e,sep}$ increases by $1.6 \times 10^{18} \text{ m}^{-3}$.

Comparison between measured and predicted Be II, W I, and W II spectral line emission demonstrates that the plasma-surface interaction model of EDGE2D-EIRENE lacks the level of detail required to predict the W line emission more accurately than an order of magnitude (Fig. 5.3). With fully predictive Be and W erosion and transport, EDGE2D-EIRENE underestimates the Be density at the low-field side target by a factor of 100 due to the lack of a Be re-erosion model. None of the deposited Be in EDGE2D-EIRENE is re-eroded, whereas in experiments Be atoms deposited in net erosion regions may be re-eroded and promptly redeposited dozens or hundreds of times before reaching a permanent deposit.

If Be atoms are injected in EDGE2D-EIRENE radially uniformly at the low-field side target to compensate for the lack of re-erosion, such that the measured Be II line emission is reproduced within 25% (Fig. 5.3a), the shape and radial extent of the predicted W I emission peak corresponds more closely to the measured W I emission (Fig. 5.3b). However, the total W I emission is underpredicted by a factor of 3, likely primarily due to the assumption of perpendicular incidence angle in the calculation of
the EDGE2D-EIRENE W sputtering rates. A more realistic incidence angle of approximately 60° (Fig. 2.3) would be a sufficient improvement to correctly predict the W I emission within the measurement and modelling uncertainties.

Despite underpredicting the W I emission by a factor of 3, EDGE2D-EIRENE overpredicts the W II emission by a factor of 4 due to neglecting W prompt redeposition (Fig. 5.3c). More than 90% of the eroded W is expected to be promptly redeposited in JET low-recycling conditions, emitting W I but unlikely to emit W II, which is why the ratio of W II to W I emission predicted by EDGE2D-EIRENE exceeds the observed W II/W I ratio by more than an order of magnitude. If the W sputtering rate in EDGE2D-EIRENE was adjusted to predict the same W I emission intensity as measured by spectroscopy, the W II emission would be overpredicted by a factor of 12. However, virtually all of the W atoms ionised near plasma-wetted surfaces, which EDGE2D-EIRENE neglects to promptly redeposit, are nevertheless locally redeposited due to the electrostatic and friction...
forces in EDGE2D-EIRENE. Therefore, inaccuracies in predicting the W I and W II emission do not imply the inability of EDGE2D-EIRENE to predict the main plasma W density.

5.2.2 W erosion in JET type-I ELMy H-mode

ERO2.0 predicts a similar intensity of W I emission (Fig. 5.4) at the JET low-field side divertor target as measured (Fig. 5.5) in JET H-mode, however the predicted W I emission is localised closer to the target than the poloidal W I emission profile reconstructed from the measurement. This could be due to the tomographic reconstruction process being unable to accurately determine the emission locations along camera lines-of-sight,
or due to neutral W being ionised closer to the surfaces in ERO2.0 than in the experiment. Agreement in the high-field side divertor is not expected due to the background plasma conditions not matching the measured conditions at the high-field side target.

Both ERO2.0 and the reconstructed measurements indicate that the W I emission at the low-field side vertical divertor (R > 2.85 m) is orders of magnitude weaker than at the strike points. However, the lack of W I emission does not imply the absence of W erosion, but is a consequence of the low electron temperature and density at the low-field side vertical divertor. The predicted W erosion source density due to CX atoms on tiles 7 and 8 is 2–3 orders of magnitude lower than due to Be ions at the low-field side strike point, but due to the large area of the low-field side vertical divertor it constitutes a non-negligible fraction (>10%) of the predicted
total W erosion rate.

The synthetic line-integrated W I emission predicted by ERO2.0 along the low-field side target is consistent with spectroscopic measurements, in terms of both the intensity and the shape of the emission peak (Fig. 5.6). The uncertainty of localising W emission in the 2D tomographic reconstruction is eliminated in the line-integrated measurements. The predicted W I intensity during ELMs is a factor of 3 higher at the strike point, and more than a factor of 10 higher when considering the entire LFS target, compared to the inter-ELM phase. The radial width of the predicted W I emission peak is narrower between ELMs and wider during ELMs, resulting in ELM-averaged emission similar to the measurement. The measured emission is also ELM-averaged due to the time resolution of the diagnostic system being lower than the ELM frequency.

The singly-ionised W II emission predicted by ERO2.0 is an order of magnitude weaker than measured (Fig. 5.7). This is partially due to the W II photon emission coefficient data used as input in ERO2.0, which is a factor of 2 lower than the W II photon efficiency for the same 434.8 nm spectral line determined from TEXTOR tokamak experiments with tungsten hexafluoride injection in similar plasma conditions. Dividing the observed factor-of-10 code-experiment discrepancy by 2, the remaining factor of 5 is presumably due to uncertainties or inaccuracies in the applied ERO2.0 models and assumptions, such as the sheath model or the assumed...
angular and energy distribution of sputtered W atoms. The ratio of W I to W II emission may also be significantly altered by the tracking of metastable W electron state populations [84], which is not included in the presented ERO2.0 simulations. The inaccuracy of singly-ionised W predictions at the low-field side target has a negligible impact on the predicted W density in the main plasma (section 5.5.2) due to the near-perfect divertor screening of W predicted by ERO2.0.

The total W erosion rate predicted by ERO2.0 during ELMs is approximately 20–30 times higher than in the inter-ELM phase (Fig. 5.8). Hybrid scenario plasmas, with up to 35 MW of heating, corner-corner configuration, and low-recycling SOL, have a several times higher predicted inter-ELM W erosion rate than the reference scenario JPN 94605–07 with 18 MW of heating, V5/C configuration, and higher recycling. The low-recycling SOL and consequently near-isothermal high electron temperature in the hybrid scenario is due to the combination of the high heating power and the corner-corner divertor configuration, which is predicted by EDGE2D-EIRENE to result in several times more effective pumping and thus lower recycling at a given D$_2$ fuelling rate, compared to the reference V5/C target configuration.

The sensitivity of the W erosion rate to the ad-hoc cross-field heat and particle transport multipliers applied during ELMs in the JINTRAC plasmas is one of the largest sources of uncertainty in the predicted ELM phase W erosion rates, as the appropriate values for the multipliers can only be loosely constrained based on the typical measured ELM energy loss and the heat loads on the divertor targets. Reducing the heat and particle
transport during ELMs by 20% results in more than 30% lower W erosion rate. Perhaps surprisingly, increasing the transport multipliers by 50% only increases the W erosion rate by 15%, because the sputtering yield of W by D ions is only weakly sensitive to the impact energy in the range of several keV (Fig. 2.3).

Increasing or reducing the heat flux entering the SOL from the core plasma, all other input parameters being equal, has a positive, stronger than linear correlation with the W erosion rate. The impact of a 20% change in the SOL heating power is 20–40% in both the ELM and inter-ELM phases. The D₂ fuelling rate has a weaker impact of 5–15% on the W erosion rate, with higher fuelling rate resulting in less W erosion due to a higher density and thus lower temperature in the SOL.

The W erosion rate in tritium plasmas is a factor of 2 higher than in deuterium plasmas, both during the inter-ELM and the ELM phase. Tritium main ions result in a 20–30% higher predicted Be concentration in the SOL than deuterium, however most of the increased W erosion in tritium was directly due to the higher W sputtering yield of T projectiles compared to D (Fig. 2.3). In the inter-ELM phase with electron temperatures below 40 eV, W sputtering by T is dominated by CX atoms, whereas during ELMs T ions are the main cause of sputtering.
5.3 Net and gross erosion of high-Z impurity markers in ASDEX Upgrade

![Figure 5.9](image)

**Figure 5.9.** Net erosion of the a) 5x5 mm and b) 1x1 mm Au marker samples, observed in the experiment and predicted by ERO. c) Gross erosion and deposition rate of Au in the $Z_{eff}=2.47$ base case (BC). Figure reprinted from Publication IV.

Experimental analysis and ERO simulations of the erosion and redeposition of Au marker samples on a Mo coating layer in ASDEX Upgrade L-mode experiments (section 4.3) were carried out to study the short-range migration of heavy impurities in the LFS divertor. Au was used as a substitute for W markers to distinguish between the marker samples and the W plasma-facing components. The net erosion rates of 5x5 mm and 1x1 mm Au marker samples predicted by ERO are qualitatively consistent with the measured erosion (Fig. 5.9). Quantitative agreement may be affected by the assumption of $T_i = T_e$ at the LFS target in the OEDGE background plasmas, among other modelling uncertainties. Net deposition peaks are predicted on both sides of the marker samples.

The electron temperature is predicted to have a larger impact on the Au net erosion rate than the electron density and the impurity concentrations. The difference in electron temperature between the base case and the high-T case is approximately 60% (25 eV and 40 eV at the strike point
Prediction and validation of heavy impurity erosion and transport respectively), and the difference in Au net erosion rate near the strike point is a factor of 2.5–3 between the two cases. The importance of the impurity concentration is predicted to be higher in regions further away from the strike point with $T_e < 20$ eV, as Au sputtering by the D main ions becomes negligible.

The predicted net erosion rate of the Mo marker layers reaches its maximum in the same location as experimentally observed, however all of the simulated scenarios underpredict the net Mo erosion rate by a factor of >3 (Fig. 5.10a). However, the Mo spectral line emission predicted by ERO is consistent with spectroscopy (Fig. 5.10c), indicating that the predicted Mo gross erosion rate is plausible. The high >90% fraction of predicted local Mo redeposition (Fig. 5.10b) may explain the low predicted net Mo erosion. Changes to the anomalous cross-field diffusivity or the electric field may result in higher migration of Mo away from the marker layers, reducing the local redeposition fraction. The impact of impurity concentration on the predicted Mo erosion rate is negligible due to D ions being the dominant cause of Mo sputtering in the studied conditions.

In a scenario with the Au marker samples replaced with W markers, and assuming no other sources of W in the plasma, the net erosion rate of the W markers is predicted to be lower than the Au markers by a factor of 3–5 (Fig. 5.11). Although Au (Z=79) is a heavier element than W (Z=74), Au is more readily eroded due to its lower surface binding energy and thus higher sputtering yields.

The typical migration distance of Au until redeposition is predicted to be in the range of several millimetres in the toroidal and poloidal directions (Fig. 5.11c), with 70% of the eroded Au being redeposited within 10 mm of the marker. The migration patterns predicted for W and Au are similar, indicating that Au markers provide a comparable substitute for W in migration experiments when W sources from other locations in the device prevent the analysis of experiments using W markers.

5.4 Divertor screening by W source location in JET

The W screening efficiency on top of the low-field side divertor entrance is several times weaker (Fig. 5.12, case 10) than in other locations in the JET divertor, based on EDGE2D-EIRENE and DIVIMP simulations with W erosion replaced by artificial atomic W sources. A W source placed near the divertor targets in the near SOL (cases 3, 6, 7) or in the far SOL (cases 1, 2, 8) results in negligible W density in the main plasma, whereas a W source of the same magnitude injecting W directly into the upstream trapping region results in 3 orders of magnitude higher main plasma W concentration (case 10). The W screening on the vertical part of the low-field side divertor entrance (case 9) is one order of magnitude better than
Figure 5.10. a) Net erosion (negative) and deposition (positive), b) gross erosion and deposition rate of the Mo marker layer, observed in the experiment and predicted by ERO. c) Measured and predicted Mo spectral line emission at 550 nm across the LFS target. Figure reprinted from Publication IV.

on the horizontal part 10 centimetres above it (case 10). A major factor contributing to the difference in W screening between cases 9 and 10 is the predicted stagnation point of the D ion flow, located near the X-point in
the near SOL and nearly halfway between the divertor entrance and the low-field side mid-plane in the far SOL. The W screening is also imperfect in the private flux region (cases 4, 5), however the private flux region is not expected to be a significant W source in experiments due to low particle and heat fluxes incident on W surfaces except near the strike points.

5.5 W density in the JET main plasma

5.5.1 W main plasma density in JET low-recycling L-mode

JINTRAC integrated core-edge modelling of W erosion and transport in low-recycling L-mode conditions, with Bohm-gyro-Bohm anomalous transport and NCLASS neoclassical transport, predicts the W density in the main plasma within measurement uncertainties of the experimentally

![Figure 5.11. Net erosion and deposition profiles of the a) 5x5 mm and b) 1x1 mm marker samples, comparing W and Au as the marker materials simulated in ERO. c) 2D profile of deposited Au particles near the 5x5 marker samples predicted by ERO in the high-T $Z_{\text{eff}}=1.66$ case. Figure reprinted from Publication IV.](image)
Figure 5.12. W density in the JET divertor predicted by EDGE2D-EIRENE with sputtering replaced by an artificial neutral W source in the locations indicated by black arrows. Sources in cases 1, 2, 8, 9, and 10 are in the far SOL, 3, 6, and 7 in the near SOL, and 4 and 5 in the private flux region. The magnitude of the W source is identical in all 10 cases to compare the screening in different parts of the divertor. The simulations are based on the inter-ELM phase of H-mode discharge #83393 with the cross-field drifts enabled. The investigation has been repeated using DIVIMP and EDGE2D-EIRENE, in L-mode and inter-ELM H-mode, with and without the drifts, with qualitatively the same results. The colour scale is logarithmic.

Figure 5.13. Flux-surface averaged main plasma W density in JET L-mode discharge #81472 (red dashed line with shaded 30% confidence intervals) and predicted by EDGE2D-EIRENE with intrinsic Be only (black line), by EDGE2D-EIRENE and DIVIMP with a 0.5% Be concentration imposed at the targets (orange solid and dashed lines respectively), by EDGE2D-EIRENE assuming zero toroidal plasma rotation (green line), and by integrated JINTRAC core-edge modelling (blue line). Figure reprinted from Publication II.
inferred W density (Fig. 5.13). The modelling uncertainties are estimated to be larger than the measurement uncertainties, which indicates that the observed level of code-experiment agreement exceeds the expectations and is not assured to remain as high in other plasma scenarios. The most significant modelling uncertainties are considered to be induced by uncertainty in the simulated main ion and electron temperature, density, and flow velocity profiles, as well as simplifications in the W core and SOL transport models. Based on the integrated modelling, both the EDGE2D-EIRENE and DIVIMP predictions of W density in the edge plasma are consistent with the experiment within a factor of 2.

5.5.2 W main plasma density in JET type-I ELMy H-mode

![Figure 5.14. Flux-surface averaged W density in JET H-mode #82486 at 14 s, calculated from diagnostics (red dashed line with shaded 30% confidence intervals), compared to code predictions. Orange solid line: EDGE2D-EIRENE with ELMs. Blue solid line: SANCO output from integrated modelling with ELMs. Purple solid and dotted line: EDGE2D-EIRENE and DIVIMP respectively without ELMs. Figure reprinted from Publication II.](image)

JINTRAC integrated modelling of W erosion and transport in intermediate-recycling type-I ELMy H-mode conditions, using the same modelling approach as for L-mode with the addition of ad-hoc descriptions of the edge transport barrier and the ELMs, overpredicts the W density in the main plasma by a factor of 2–4 (Fig. 5.14). The modelling represents an inter-ELM end state following multiple ELM cycles, continued until an approximate periodic steady state is reached, whereas the experimentally inferred W density profile is ELM-averaged. The main source of inaccuracy in the JINTRAC predictions is suspected to be the simulated edge transport barrier properties, which were not sufficiently accurately constrained by measurements of the electron density and temperature gradients in the edge of the main plasma. The high electron density gradient in JINTRAC
induces strong convective inward neoclassical transport of W into the pedestal top, resulting in a very high W density gradient and a pedestal W density exceeding the experimentally inferred value by a factor of 4. The accuracy of the JINTRAC predictions in Fig. 5.14 could potentially be improved by more thorough validation of the simulated gradients in the background plasma conditions and by applying a more comprehensive neoclassical impurity transport model such as NEO.

Comparison of EDGE2D-EIRENE predictions of the main plasma W density with and without type-I ELMy densities indicates that the higher W erosion rate during ELMy plasmas results in a several-fold increase in the ELM-averaged main plasma W density (Fig. 5.14). Modelling a single ELM cycle characterises the predicted erosion, SOL transport, and deposition of W, whereas predicting the W density in the main plasma requires simulating multiple consecutive ELM cycles. The extrapolation of the experimentally inferred W core plasma density to the edge plasma suggests that ELM-free EDGE2D-EIRENE simulations potentially underpredict the pedestal W density by a factor of 3–6 in intermediate-recycling H-mode conditions with 10 MW of auxiliary heating.

Predictions of the main plasma W density in JET type-I ELMy H-mode discharges with 18–35 MW of heating, using ERO2.0 for W erosion and edge transport, and JETTO+SANCO with NEO neoclassical transport for core W transport, agree with the experimentally inferred W density within approximately a factor of 2 at all locations within the main plasma (Fig. 5.15 and Fig. 5.16). Both ERO2.0 and JINTRAC predict the poloidal distribution of W to be roughly similar to the observed W asymmetry along the closed flux surfaces, driven primarily by the toroidal rotation of the plasma. A radially constant rotation frequency was assumed, corresponding to the frequency measured at the ERO2.0 core boundary and overestimating the rotation at the separatrix, which is why ERO2.0 predicts the W density near the separatrix to be more localised to the LFS mid-plane compared to NEO and the experiment. The ERO2.0 simulations represent the inter-ELM phase with W erosion enabled in the low-field side vertical divertor only, to save the computational cost of simulating W erosion and local redeposition in regions which contribute negligible influx of W to the main plasma. The boundary condition for W density in the JINTRAC simulations has been adjusted to approximately reproduce the flux-surface-averaged W density predicted by ERO2.0 at the pedestal top (normalised minor radius 0.9). The level of agreement between the code predictions and the experiment is within the modelling uncertainties in both of the studied scenarios. Compared to Fig. 5.14, the improved code-experiment agreement is primarily due to more thorough validation of the simulated plasma conditions, particularly in the pedestal and the edge transport barrier, as well as due to NEO being a more appropriate W transport model than NCLASS.
Figure 5.15. Poloidal cross-section of the W density in the main plasma of JPN 94606 at 10 s a) inferred from experiment, b) predicted by JINTRAC with NEO, c) predicted by ERO2.0. All three figures share the same colour scale.
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Figure 5.16. Poloidal cross-section of the W density in the main plasma of JPN 97781 at 8 s a) inferred from experiment, b) predicted by JINTRAC with NEO, c) predicted by ERO2.0. All three figures share the same colour scale.
5.5.3 Impact of SOL electron density and temperature on the main plasma W concentration

The W concentration in the main plasma is a strongly increasing function of the electron temperature at the divertor targets and a strongly decreasing function of the upstream electron density (Fig. 5.17). Although the electron temperature at the strike points is one of the most critical parameters in determining the total gross W erosion rate, the direct causal connection between W erosion rate in the divertor and the main plasma W concentration is predicted to be very weak. Instead, the main plasma W concentration is largely determined by W erosion due to charge-exchange atoms on poorly screened W surfaces (section 5.4), and by W transport in the SOL and main plasma. The presented results are an update to earlier EDGE2D-EIRENE predictions [85], improved with several bug fixes to the EDGE2D-EIRENE plasma-surface interaction model as well as a more realistic beryllium concentration in the divertor.

Comparison of the W concentration predicted in L-mode (Fig. 5.17a) and inter-ELM H-mode (Fig. 5.17b) indicates that the SOL regime (sec-
tion 2.1.4) is a more relevant parameter for determining the W concentration than the absolute value of electron density or temperature in the SOL. DIVIMP consistently predicts approximately 50% higher W concentration than EDGE2D-EIRENE in attached plasmas. This is mostly due to the effect of W charge state bundling in EDGE2D-EIRENE (section 5.1).

5.5.4 Impact of W anomalous cross-field diffusivity on the W content

![Figure 5.18. Total W content within the closed flux surfaces predicted by EDGE2D-EIRENE as a function of the assumed W cross-field diffusion coefficient in JET L-mode. The plasma conditions are based on JPN 81472 at 10 s.](image)

While the anomalous cross-field diffusivity $D_\perp$ of the main ions can be inferred experimentally from the observed density gradients, assuming the ion sources and sinks and the neoclassical transport are known, the anomalous diffusivity of impurities is more difficult to determine. First-principles anomalous transport codes such as QuaLiKiz (section 4.2.3) can predict $D_\perp$ for all plasma species, but the validation of such predictions for impurities is challenging due to a lack of applicable measurements. Hence, predicting the main plasma impurity density within reasonable uncertainty is only possible if the impact of impurity $D_\perp$ on the predictions is proven to be sufficiently weak.

Assuming purely diffusive cross-field transport, the W content in the main plasma is a weakly decreasing function of the $D_\perp$ of W (Fig. 5.18) based on EDGE2D-EIRENE predictions in JET L-mode plasmas. The $D_\perp$ of W has a negligible impact on the W erosion rate (Fig. 5.8), which implies that the increased W content at lower $D_\perp$ is entirely due to a longer average dwell time of W in the main plasma. Knowing $D_\perp$ within the correct order of magnitude is sufficient to determine the W content within
Prediction and validation of heavy impurity erosion and transport

If neoclassical convection is included in the cross-field transport model, the predicted W content in the limit of low $D_\perp$ becomes highly sensitive to the direction of the convective velocity. In typical H-mode edge transport barriers, anomalous transport is suppressed and the normalised density gradient is high, implying low $D_\perp$ and strong inward convection of W. Thus, large W density gradients are expected within the transport barrier. On the other hand, diffusive cross-field transport of W has been found a reasonable approximation at the pedestal top even in H-mode [40].

5.5.5 Impact of cross-field drifts on W transport

EDGE2D-EIRENE predicts that the inclusion of drifts does not significantly affect the total W content in the main plasma in low-recycling, non-rotating L-mode plasma conditions (Fig. 5.19). However, the drifts induce a top-down W asymmetry in the main plasma. The W density is predicted to vary by up to a factor of 3–4 in the poloidal direction and reach its maximum near the lowest point of each flux surface. In JET L-mode plasma experiments heated by neutral beam injection, no such top-down asymmetry is observed experimentally as the highest W density is located near the LFS mid-plane due to the rotation of the plasma (section 5.5.6). Both the EDGE2D-EIRENE background plasmas with and without drifts are consistent with the measured upstream and target electron density and temperature profiles in this low-recycling L-mode scenario, indicating
that the drifts are not necessary to obtain validated background plasmas in these conditions. However, drifts potentially have a significant effect on the flow velocity profile of the main ions in the SOL, which greatly affects W via the frictional force; the flow velocity profiles of the main ions are not measured in JET. Thus, the inclusion of drifts in the background plasma simulations can be expected to improve the prediction accuracy of W transport even if the drift background plasma is equally accurate as the no-drift plasma when validated against measurements.

DIVIMP predicts that the inclusion of the $\vec{E} \times \vec{B}$ drift acting on W in a high-recycling, non-rotating, inter-ELM H-mode background plasma with cross-field drifts enabled, causes a reduction in the predicted main plasma W density by a factor of 2–3 (Fig. 5.20b,d). In a background plasma without drifts, the $\vec{E} \times \vec{B}$ drift on W is predicted to change the peak location of W accumulation from the LFS to the top of the plasma near the separatrix (Fig. 5.20a,c). Only the $\vec{E} \times \vec{B}$ drift is implemented in DIVIMP, which means that the impact of other drifts, such as the grad-$\vec{B}$ drift, acting on W is neglected in these predictions.

Separating the background plasma modelling (EDGE2D-EIRENE) from the W transport (DIVIMP) enables the independent analysis of cross-drift effects directly on W and indirectly via the altered plasma conditions. The drifts have a critical impact on the predicted SOL conditions in the studied background plasma, changing the SOL from low-recycling to the high-recycling regime. Thus, the drifts reduce the electron temperature and increase the electron density by several times at both divertor targets, thereby reducing the total W erosion rate by an order of magnitude. The background plasma with drifts is consistent with the measured upstream and target plasma conditions, unlike the no-drift background plasma.

The drifts are predicted to have a larger impact in the presented high-recycling H-mode scenario than in most other scenarios, due to the combination of the high radial gradients in H-mode and the high sensitivity of the divertor plasma to the upstream conditions in the high-recycling regime. Unlike the presented scenario with target conditions strongly diverging between the drift and no-drift simulations, no-drift background plasmas which are validated against both upstream and target conditions are expected to yield W predictions which do not drastically differ from plasmas with drifts and similar plasma conditions as the no-drift plasmas.

5.5.6 Impact of toroidal plasma rotation on the W density profile

EDGE2D-EIRENE predictions of the HFS-LFS W density asymmetry agree with the experimentally inferred W profile within a factor of 2 in JET L-mode (Fig. 5.21), when the toroidal rotation of the plasma is accounted for by imposing a boundary condition for the main ion and impurity parallel-\(B\) flow velocity at the core boundary in EDGE2D-EIRENE. If the flow
Figure 5.20. Poloidal cross-section of the W density in steady inter-ELM H-mode based on JPN 83393 at 21 s predicted by DIVIMP a) with no cross-field drifts affecting the background plasma or W transport, b) drifts affecting the background plasma but not W, c) drifts affecting W but not the background plasma, d) drifts affecting both W and the background plasma.
velocities are set to zero at the core boundary, EDGE2D-EIRENE predicts virtually no W asymmetry in the main plasma unless cross-field drifts are enabled.

DIVIMP does not contain an implementation of the centrifugal effect, which is why DIVIMP predicts an opposite HFS-LFS W asymmetry compared to EDGE2D-EIRENE and the experimental observations (Fig. 5.21). The W asymmetry predicted by DIVIMP is driven by the parallel-B force balance model (equation 2.14), which leads to the W density peaking near the HFS mid-plane separatrix.

ERO2.0 predicts that the main plasma W density profile becomes increasingly localised to the LFS mid-plane as the assumed toroidal rotation frequency of the plasma is increased (Fig. 5.22). Toroidal plasma rotation also has a noticeable effect on the parallel-B force balance in the SOL in inter-ELM H-mode, reducing the predicted W accumulation near the HFS mid-plane separatrix. In a non-rotating background plasma, the predicted poloidal W asymmetry driven by neoclassical transport on closed flux surfaces is significantly weaker and opposite to the rotation-driven asymmetry. The neoclassically driven W asymmetry also contains a top-down component, with several times higher W density at the top of the main plasma than near the X-point (Fig. 5.22a).
Figure 5.22. W density in JPN 94606 at 10 s predicted by ERO2.0 a) without the centrifugal effect, b) assuming a toroidal rotation frequency of $10^4$ rad/s, c) rotation frequency $2 \cdot 10^4$ rad/s.
6. Conclusions

This thesis provides the first demonstrations of the ability of fully predictive W erosion and transport simulations in validated background plasmas to forecast the W density in the JET main plasma within a factor of 2 of the experimentally inferred W density, in plasma scenarios ranging from L-mode to the highest-performance type-I ELMy H-mode discharges. A novel modelling approach combining the simulation tools EDGE2D-EIRENE and ERO2.0 with JINTRAC and NEO is presented and validated, and the uncertainties in the models assessed. The ability to predict W erosion and transport is critical to designing fusion devices with W plasma-facing components, due to the implications on plasma performance and on the lifespan of wall components.

ERO2.0 predictions of W erosion in JET type-I ELMy H-mode plasmas are consistent with the measured neutral tungsten spectral line emission within the modelling uncertainties in the low-field side divertor. However, ERO2.0 is found to underpredict the singly ionised tungsten emission by a factor of 10, partially due to uncertainty in the assumed W photon emissivity coefficients. EDGE2D-EIRENE simulations predict lower-than-measured neutral W emission by a factor of 3 in the low-field side divertor, likely due to the assumption of a perpendicular ion impact angle. Due to neglecting prompt redeposition, EDGE2D-EIRENE nevertheless overpredicts the singly-ionised W emission by a factor of 4.

Although the divertor targets are the largest gross source of W in JET L-mode and H-mode plasmas, the W erosion rate predicted at the divertor targets has a negligible impact on the predicted main plasma W density due to virtually perfect divertor screening. The majority of the predicted W sputtering at the targets is promptly redeposited, and nearly all of the W near the targets is locally redeposited due to the combination of the pre-sheath electric field and the flow of the main ions, even if prompt redeposition is neglected. The EDGE2D-EIRENE, DIVIMP, and ERO2.0 predictions indicate that the W influx into the JET main plasma is primarily from W erosion by charge-exchange atoms near the low-field side divertor entrance. The predicted W screening efficiency of plasma-facing
components on the LFS between the X-point and the mid-plane is several orders of magnitude lower than at the divertor targets.

Integrated core-edge JINTRAC simulations of W erosion and transport, using EDGE2D-EIRENE for W erosion and SOL transport, and Bohm-gyro-Bohm and NCLASS for core W transport, predict the main plasma W density within measurement uncertainties in L-mode plasmas. In type-I ELMy H-mode, significant uncertainty induced by the assumed ELM and edge transport barrier properties results in the JINTRAC-predicted W density exceeding the inferred total W density in the main plasma by a factor of 2–4.

Based on the parameter sensitivity studies conducted in this thesis, the combined uncertainty of W erosion and transport predictions in fully predictive H-mode background plasmas is expected to be higher than a factor of 3, but potentially less than a factor of 10 in non-pathological cases with approximately correct background plasma predictions. Reducing the predictive uncertainty of the W density in future devices requires new advances in predicting the background plasma conditions both in the SOL and in the core plasma. The critical SOL parameters to predict include the electron density and temperature profiles, the ion flow velocity pattern, the energy-resolved atomic flux density, and the time-resolved ELM dynamics. On the closed flux surfaces, accurate radial ion temperature and density gradients, especially in the edge transport barrier, and the toroidal rotation frequency are necessary for accurate predictions of the W density.

In addition to the uncertainty induced by the background plasma conditions, the assumptions and approximations of the W transport models, as well as the atomic data for calculating reaction rates such as sputtering and ionisation, contribute to the uncertainty of W erosion and transport predictions in both predictive and thoroughly validated background plasmas. The exact contribution of each uncertainty source is difficult to isolate by code-experiment comparisons due to incomplete diagnostic coverage of the charge-resolved W density at every location in the plasma. However, a lower bound of a factor of 2 is estimated for the uncertainty of the most complete description of W erosion and transport in JET type-I ELMy H-mode presented in this thesis, based on validated EDGE2D-EIRENE background plasmas, ERO2.0 for W erosion and edge transport, and JINTRAC with NEO for W core plasma transport. The W predictions obtained using this modelling approach are within the estimated factor-of-2 uncertainty of the experimentally inferred W density in all of the studied plasma scenarios, including the 2D poloidal main plasma W density profile, with the exception of the W II emission at the LFS target which has a negligible impact on the predicted main plasma W density.

EDGE2D-EIRENE is found to consistently predict a lower W density than DIVIMP by one-third in the main plasma compared to DIVIMP, in both L-mode and inter-ELM H-mode plasmas, across a wide range of
electron densities and temperatures in attached plasma conditions. The bundling of the 74 W ionised charge states into 6 fluid species in EDGE2D-EIRENE reduces the average charge of W in the SOL, leading to weaker parallel-B forces and less accumulation of W in the upstream. Increasing the number of fluid species in EDGE2D-EIRENE is not a feasible solution despite correctly predicting the W charge, because it results in large numerical inconsistencies in EDGE2D-EIRENE violating the conservation of W momentum and thus unphysical W transport. Additionally, an excessive number of fluid species leads to a low probability of a converged EDGE2D-EIRENE solution. The presented simulations suggest that the EDGE2D-EIRENE W density predictions may be adjusted to account for the W bundling effect by multiplying the W density in the JET main chamber by a scaling factor of 1.5. When feasible, using EDGE2D-EIRENE to model only the background plasma conditions, and applying a more comprehensive physics model such as ERO2.0 for W erosion and SOL transport, is advantageous for reducing the modelling uncertainties.

Predictive ERO simulations of the net and gross erosion of Au marker samples on a Mo substrate in ASDEX Upgrade, to investigate small-scale, local migration of heavy impurities, qualitatively reproduce the observed net erosion rate of Au. The electron temperature was identified as the most significant parameter in determining the predicted Au erosion rate. The predicted Mo spectral line emission is consistent with spectroscopic measurements, indicating a realistic Mo gross erosion rate despite ERO underestimating the measured net Mo erosion by a factor of >3. The migration behaviour of eroded Au and W is predicted by ERO to be similar, with the exception of the 3–5 times higher sputtering yield of Au compared to W. The ERO simulations suggest that Au marker samples are a feasible proxy for experimental W erosion and migration studies when W sources from other W plasma-facing components complicate the analysis of measured W marker erosion. The findings from the ASDEX Upgrade Au marker studies are expected to be applicable to any tokamak with a W divertor and comparable attached L-mode plasma conditions.

In future fusion reactors which are expected to achieve detachment by impurity (e.g. neon) seeding, the seeded impurities have been predicted to increase the W erosion rate at low seeding rates and incomplete detachment, but decrease W erosion when the seeding rate is sufficient to significantly reduce the electron temperature at the divertor targets [86]. The issues of W erosion and plasma contamination by W are mitigated by fully detached plasma scenarios, however it will be determined whether such detached scenarios are compatible with simultaneous high fusion performance. If the scenario involves type-I ELMs with ion impact energies in the several keV range, seeded Ne or N ions surpass T+ as the dominant cause of gross W erosion at impurity concentrations $\gtrsim 2–4\%$ [87]. Nevertheless, if the divertor screening at the targets is as efficient as predicted
by the JET simulations in this thesis, W erosion by seeded impurity ions is unlikely to cause intolerable W contamination of the main plasma.
References


References


Appendix A: Validation of the simulated background plasmas
Figure 6.1. Ion and electron cross-field heat and particle diffusion coefficients (a, d) used in EDGE2D-EIRENE to reproduce the electron density and temperature profiles measured by high-resolution Thomson scattering, Li-beam, and reciprocating probe along the LFS mid-plane (b, c, e, f) in the L-mode JPN 81472 at 9 s (a–c) and JPN 82486 inter-ELM H-mode at 14 s (d–f) scenarios. (Publication II)
Figure 6.2. Electron temperature (a, c) and density (b, d) profiles predicted by EDGE2D-EIRENE (solid lines) compared to Langmuir probe (LP) measurements (markers) along the LFS target in the L-mode JPN 81472 at 9 s (a, b) and inter-ELM H-mode JPN 82486 at 14 s (c, d) scenarios. The LP data are limited to a maximum of 100 eV and thus are not shown for the intra-ELM conditions. (Publication II)
Appendix A: Validation of the simulated background plasmas

Figure 6.3. Comparison of Langmuir probe measurements and predicted EDGE2D-EIRENE plasma conditions with (black solid lines) and without (red solid lines) cross-field drifts along the LFS target in low-recycling L-mode based on JPN 81472 at 9 s (a, b) and high-recycling inter-ELM H-mode based on JPN 83393 at 21 s (c, d).
Figure 6.4. Electron density and temperature profiles along the low-field side mid-plane measured by HRTS (blue and red markers and fitted lines) and simulated in EDGE2D-EIRENE (black lines), JPN 94605 pre-ELM conditions at 10 s. (Publication III)

Figure 6.5. Ion temperature profile along the low-field side mid-plane from EDGE2D-EIRENE (black line) and measured by CXRS (markers), JPN 94605 at 10 s. (Publication III)
Appendix A: Validation of the simulated background plasmas

Figure 6.6. Electron density, electron temperature, and ion saturation current profiles measured by Langmuir probes (markers) and predicted by EDGE2D-EIRENE (black lines) along the low-field side divertor target, JPN 94605 at 10 s. Dotted lines: +/-20% variation in the heat flux entering the edge plasma, dashed lines: +/-20% variation in the D\textsubscript{2} fuelling rate in EDGE2D-EIRENE. (Publication III)

Figure 6.7. Time evolution of the pedestal electron temperature from EDGE2D-EIRENE (black line) and measured by different channels of electron cyclotron emission (dashed lines), JPN 94605 at 10 s. (Publication III)
Appendix A: Validation of the simulated background plasmas

Figure 6.8. Time evolution of plasma stored energy from EDGE2D-EIRENE (black line) with arbitrary offset to account for the partially missing core region, and measured by magnetic equilibrium reconstruction (blue dashed line), JPN 94605 at 10 s. (Publication III)

Figure 6.9. Time evolution of the ELM power load on the low-field side target from EDGE2D-EIRENE (black line) and measured by infrared cameras (blue line), JPN 94605 at 10 s. (Publication III)
Appendix A: Validation of the simulated background plasmas

Figure 6.10. Electron density profile in the core plasma from JETTO (black line) and measured by HRTS (markers), JPN 94606 at 10 s.

Figure 6.11. Ion temperature profile in the core plasma from JETTO (black line) and measured by CXRS (markers), JPN 94606 at 10 s.
Appendix A: Validation of the simulated background plasmas

Figure 6.12. Electron density and temperature profiles along the low-field side mid-plane from EDGE2D-EIRENE (black line) and measured by HRTS (blue and red markers and fitted lines), JPN 96947 at 8 s. (Publication III)

Figure 6.13. Ion temperature profile along the low-field side mid-plane from EDGE2D-EIRENE (black line) and measured by CXRS (markers), JPN 96947 at 8 s. (Publication III)
Figure 6.14. Electron density profile in the core plasma from JETTO (black line) and measured by HRTS (markers), JPN 97781 at 8 s.

Figure 6.15. Toroidal rotation velocity profile in the core plasma from JETTO (black line) and measured by integrated data analysis of impurity diagnostics (markers), JPN 97781 at 8 s.
Figure 6.16. Electron temperature profile in the core plasma from JETTO (black line) and measured by HRTS (markers), JPN 97781 at 8 s.

Figure 6.17. Ion temperature profile in the core plasma from JETTO (black line) and measured by CXRS (markers), JPN 97781 at 8 s.
Figure 6.18. a) Electron temperature and b) electron density profiles along the LFS target in ASDEX Upgrade, used as boundary conditions of the OEDGE background plasmas, compared to Langmuir probe measurements of AUG discharge #35617. c) Weighted sputtering yield of gold predicted by ERO for different B, C, and N concentrations corresponding to effective charges $Z_{eff} = 1.93$ and $Z_{eff} = 2.47$. (Publication IV)