Energetic particles in reactor-relevant plasmas: modelling and validation

Jari Varje
Energetic particles in reactor-relevant plasmas: modelling and validation

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Abstract

Nuclear fusion is a promising future energy source with few carbon dioxide emissions and nearly limitless source of fuel in heavy isotopes of hydrogen. Energetic particles, such as fusion-born alpha particles and neutral beam injected (NBI) fast ions play a vital role in reactor-relevant fusion plasmas, as they are responsible for heating the plasma, but can simultaneously cause localized heat loads and risk of damage on the plasma facing components. In this work, the Monte Carlo orbit-following code ASCOT has been used to simulate fast ions both to validate simulation results with present-day experiments at the JET tokamak, and to predict fast ion losses in next-generation fusion reactors ITER and DEMO.

For validation of ASCOT predictions against JET plasmas, synthetic diagnostics were used to compare the simulated fast ion distributions with the neutral particle analyser (NPA) and fast ion loss detector (FILD) measurements. The NPA simulations qualitatively reproduced the experimentally measured slowing-down distributions and fast ion isotope fraction for NBI-injected hydrogen and deuterium ions, while the FILD simulations for fusion product losses were within 10% of the experimentally observed losses.

For predictions in ITER plasmas, simulations with resonant magnetic perturbations showed that including the response of the plasma to the external perturbations is vital, as the response not only affected the magnitude but also the distribution of fast ion losses. For DEMO plasmas, the sensitivity of fast ion losses due to various magnetic perturbations was studied, including the toroidal field ripple and ferritic inserts in various configurations. The design was found to be robust with respect to fast ion confinement and losses.

Finally, over the course of this work, a highly parallelized version of the ASCOT code, called ASCOT5, was developed. The new version substantially increased the performance on modern supercomputer hardware as well as improving its maintainability and extensibility.

Keywords  plasma physics, tokamaks, fast ions, synthetic diagnostics

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ITER-reactorille tehdyt simulatiolat resonanttien magneettisten häiriöiden kanssa osoittivat, että plasman vasteen huomioiminen on tärkeää, koska se vaikuttaa niin nopeiden hiukkasten häviöiden määrään kuin jakauman reaktorin sisäseinällä. DEMO-reactorille tutkiitiin häviöiden herkkyyttä muun muassa toroidaalisen kentän eli jonkun ja ferriittisten komponenttien aiheuttamille magneettisille häiriöille. Suunniteltu reaktorigeometria osoittautui kestäväksi nopeiden hiukkasten aiheuttaman tehokuorman kannalta.

Työn aikana kehitettiin myös uusi, rinnakkaislaskentaa tehokkaasti hyödyntävä koodiversio ASCOT5. Uusi versio lisäsi suorituskykyä merkittävästi uusimmilla supertietokoneilla sekä paransi koodin ylläpidettävyyttä ja laajennettavuutta.

Avainsanat
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Preface

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Parts of the work was carried out using the HELIOS supercomputer system at International Fusion Energy Research Centre, Aomori, Japan, under the Broader Approach collaboration between Euratom and Japan, implemented by Fusion for Energy and JAEA. Parts of the work were carried out on the EUROfusion High Performance Computer (Marconi-Fusion). The supercomputing resources of CSC—IT center for science were utilised in the studies. Some of the calculations were performed using computer resources within the Aalto University School of Science “Science-IT” project.

Abingdon, United Kingdom, January 28, 2022,

Jari Varje
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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: “High-performance orbit-following code ASCOT5 for Monte Carlo simulations in fusion plasmas”

J. Varje wrote the initial implementation of the code, performed the simulation and performance benchmarks, and wrote chapters 1, 3, 4.2, 5 and 6 of the manuscript. K. Särkimäki performed the theoretical benchmarks and wrote chapters 2 and 4.1 of the manuscript. J. Varje, K. Särkimäki, J. Kontula, P. Ollus, T. Kurki-Suonio, A. Snicker, E. Hirvijoki and S. Äkäslompolo further developed the code with various models and interfaces.

Publication II: “Synthetic NPA diagnostic for energetic particles in JET plasmas”

J. Varje implemented the simulation model, prepared, performed and analysed the simulations and wrote the manuscript. P. Sirén and H. Weisen provided the experimental JET data for the simulations.

Publication III: “Synthetic diagnostic for the JET scintillator probe lost alpha measurements”

J. Varje implemented the simulation model, prepared, performed and analysed the simulations and wrote the manuscript. V. Kiptily provided information on the JET FILD geometry and relevant experiments for study. P. Sirén and H. Weisen provided the experimental data for the simulation inputs.
Publication IV: “Effect of plasma response on the fast ion losses due to ELM control coils in ITER”

J. Varje prepared, performed and analysed the simulations and wrote the manuscript. J. Varje, O. Asunta, E. Hirvijoki, T. Koskela, T. Kurki-Suonio, S. Sipilä, A. Snicker, K. Särkimäki and S. Äkäslompolo developed the framework and methods for the ITER simulations. M. Cavinato, M. Gagliardi, Y. Liu, V. Parail and G. Saibene provided input data from ITER and F4E for the simulations.

Publication V: “Sensitivity of fast ion losses to magnetic perturbations in the European DEMO”

J. Varje prepared and performed and analysed the simulations and wrote the manuscript. T. Kurki-Suonio, A. Snicker and K. Särkimäki provided input from earlier work. J. Varje, P. Vincenzi, P. Agostinetti and P. Sonato prepared the model for the DEMO NBI geometry. E. Fable provided the kinetic profiles and equilibrium. F. Villone provided the geometry for the DEMO magnetic configuration.

S. Sipilä et al. ASCOT orbit-following simulations of ion cyclotron heating with synthetic fast ion loss diagnostic: a first application to ASDEX Upgrade, Nuclear Fusion 61 086026, 2021.


Y. Kazakov et al. Plasma heating and generation of energetic D ions with the 3-ion ICRF + NBI scenario in mixed H-D plasmas at JET-ILW. Nuclear Fusion 60 112013, 2020.


P. Vincenzi et al. Estimate of 3D wall heat loads due to Neutral Beam


P. Sirén et al. Versatile fusion source integrator AFSI for fast ion and neutron studies in fusion devices, Nuclear Fusion 58 016023, 2018.


T. Kurki-Suonio et al. Effect of the European design of TBMs on ITER wall loads due to fast ions in the baseline (15 MA), hybrid (12.5 MA), steady-state (9 MA) and half-field (7.5 MA) scenarios, Nuclear Fusion 56 112024, 2016.


1. Introduction

The growing population of our planet and the increasing standards of living put ever increasing demands on energy sources, while environmental pressure, including anthropogenic climate change, acts to restrict them. Responding to these demands requires fundamentally new types of energy sources, as existing solutions are either detrimental to the environment due to CO$_2$ emissions in the case of fossil fuels, or insufficient in capacity and availability due to their variable nature in the case of solar and wind power [1]. Nuclear fission, while low in carbon emissions and high in availability, is hindered by political uncertainty and the outstanding issue of long-term high-level radioactive waste [2].

Nuclear fusion energy, on the other hand, is an alternative energy source with few drawbacks and great advantages over aforementioned energy sources. Research and development over the past fifty years have resulted in a steady increase in performance, and the next generation of devices is expected to produce net energy for the first time. The promises of nuclear fusion are great: a nearly limitless source of fuel in heavy isotopes of hydrogen, with few carbon dioxide emissions as no fossil fuels are consumed, and no high-level waste.

Yet the remaining challenges appear nearly as great: open questions remain in the physics understanding of operating fusion reactors in self-sustaining burning plasma conditions, which lies beyond the experience in present day devices. Likewise, designing reactors that can tolerate the unprecedented power loads in power plant operation requires careful predictive analysis. Experimental research and computer modelling are actively used to answer these questions, and this thesis aims to address these issues in the context of energetic particles and plasma heating in reactor-relevant devices.
Introduction

1.1 Nuclear fusion and tokamaks

Nuclear fusion is based on nuclear reactions between light nuclei fusing into heavier nuclei and releasing energy in the process. The most common reactions envisaged for fusion reactors are based on the fusion of deuterium and tritium isotopes of hydrogen

\[
D + D \rightarrow ^3He + n \quad (1.1) \\
D + D \rightarrow T + p \quad (1.2) \\
D + T \rightarrow ^4He + n \quad (1.3)
\]

The D-T reaction 1.3 is particularly enticing as it is the one with the highest cross section at the lowest temperatures (figure 1.1), making it the most practical reaction for the first generation of fusion power plants. While deuterium is abundantly available in seawater, tritium is a radioactive isotope with a half-life of 12.5 years. It can, however, be produced from isotopes of lithium, a common element in Earth’s crust and seawater, through neutron bombardment in the reactor environment.

The D-D reactions 1.1 and 1.2, on the other hand, are commonly used in existing experimental devices due to lack of radioactive tritium and reduced neutron activation, while still producing plasmas similar to those in fusion reactors. Additionally, future generations of fusion reactors could primarily use this reaction, removing the issues with tritium altogether.

Achieving nuclear fusion requires overcoming the electrostatic Coulomb potential between the two positively charged nuclei. This requires sufficient energy for the particles and thus a high ion temperature for the

Figure 1.1. Fusion cross sections for reactions between deuterium and tritium [3].
plasma. At these temperatures, the gases are fully ionized plasmas, which must be confined for the reactions to occur. The most promising method is magnetic confinement fusion, and in particular the tokamak.

Tokamaks are based on the idea of confining the charged particles in a plasma using magnetic bottle in the shape of a torus, where the charged ions follow the closed field lines in helical trajectories due to the Lorentz force. This is achieved by externally applying a toroidal magnetic field using a set of toroidal field coils (figure 1.2). Additionally, a toroidal current is driven in the plasma using the transformer principle with a set of inner poloidal field coils. This has the effect of producing a poloidal magnetic field, resulting in a helical magnetic field in the plasma. This is done to produce a rotational transform, that is needed to cancel out separation of positively and negatively charged particles, which otherwise occurs due to drifts resulting from gradients in the magnetic field.

1.2 Present and future fusion machines

In the course of development fusion power, the experimental devices have grown in size and performance. The largest currently operating machine is the Joint European Torus (JET) in the United Kingdom. It is also the only current device capable of operating with the reactor-relevant D-T mixture. This makes it an important tool in validation of the theories and models on which the design of future devices is based.

The next step after JET is the ITER thermonuclear reactor, currently being constructed under an international collaboration in France. ITER is
planned to produce a factor of 10 net gain in fusion power in its baseline operating scenario, defined as the fraction of output fusion power to input auxiliary heating power. Twice as large in scale, and with more than twice the auxiliary heating power of JET, ITER is projected to produce a total of 500 MW of fusion power. It will provide an important testbed for testing solutions and technologies for eventual power plants, including experiments for materials, power exhaust and steady-state operation.

Beyond ITER, the natural next step is a prototype fusion power plant. In Europe this is called DEMO, and it will demonstrate the engineering solutions needed for an operating power plant, with net electricity output into the grid. As currently envisioned, the device will be another 30% larger than ITER, with a planned thermal power of 2 GW, producing approximately 500 MW of electricity. DEMO will also demonstrate other key concepts of commercial operation such as breeding the tritium fuel as well as remote handling and maintenance.

1.3 Energetic particles in reactor-relevant plasmas

Energetic particles play a vital role in reactor-relevant fusion plasmas. They are responsible for maintaining sufficient conditions for fusion reactions by depositing their energy in and heating up the plasma as well as helping maintain the plasma current and momentum. At the same time, they can drive various instabilities with deleterious effect on plasma performance and cause localized heating on the plasma facing components of the device if they escape the magnetic confinement. Sources of energetic particles include the fusion reactions themselves, such as in the case of the 3.5 MeV alpha particles produced in D-T fusion, and externally produced fast ions, such as fast ions produced by neutral beam injection (NBI) or ion cyclotron resonance heating (ICRH). The energies of these particles can range from tens of keV to several MeV.

The generation mechanisms of these fast ions are well understood. However, detailed understanding of their behaviour in the plasma is vital for operation and control of any fusion reactor due to their central role in plasma heating and machine protection. Measuring the properties of these particles, determined by their distribution function, is difficult. Only limited diagnostic methods, including fast ion D-alpha (FIDA) [5], collective Thomson scattering (CTS) [6], neutral particle analysis (NPA) [7], fast ion loss detectors (FILD) [8], and neutron [9] and gamma spectroscopy [10], are available. Even then, inferring the underlying fast ion distributions is complicated. Modelling the behaviour of these particles with computational codes, applying theoretical models in realistic representations of the plasma, is needed to gain insight into the processes affecting the fast ions. Simulation predictions are also the only means to study planned future
reactors, such as ITER and DEMO.

In this work, the primary tool for studying energetic particles is the orbit-following code ASCOT [11]. The code simulates the behaviour of fast ions using the Monte Carlo method of following the trajectories of test particles in a realistic geometry, which enables detailed study of the distribution of the ions as well as power losses and heat fluxes to the reactor structures. Additional codes, based on ASCOT, are used to calculate high-fidelity fast ion sources. For NBI ions, the markers are generated using the beam ionisation code BBNBI [12], while fusion product sources can be simulated using the fusion source code AFSI [13]. Synthetic diagnostics have been developed to predict diagnostic signals based on the simulations, which can then be compared with experimental results.

To gain confidence in the predictions of simulations for future fusion experiments and reactors, the codes should be thoroughly validated with experimental data in existing devices. Such work has previously been carried out using various fast ion diagnostics, in particular at the ASDEX Upgrade tokamak [14, 15, 16, 17]. In this work, the validation of the ASCOT code is further extended by modelling fast ion diagnostics in the JET tokamak. Of particular interest is the neutral particle analyser (NPA), for which previous simulation results at ASDEX Upgrade have proven unsatisfactory, and the scintillator probe/fast ion loss detector (FILD).

The research questions that this dissertation aims to answer are:
1. What is the predicted behaviour of energetic particles in the next generation fusion reactors?
2. How reliable are these predictions, based on validation of the tools in existing reactor-relevant experiments?

The dissertation is structured as follows: The second chapter introduces fast ions in plasmas, their sources and the diagnostics used to measure their properties. Chapter 3 describes the computational tools developed for and used in the simulations and analysis in the following chapters. Chapter 4 presents validation of the codes using synthetic fast ion diagnostics in recent experimental campaigns in JET, while chapter 5 addresses the issue of fast ion confinement and losses in ITER and DEMO under various magnetic perturbations that can be expected in these devices. Finally, chapter 6 summarizes the results and presents an outlook on future research prospects.
2. Fast ions in plasmas

Fast ions represent an important population of particles in fusion plasmas. They can be characterized by their suprathermal energy $E >> T_i$, which distinguishes them from the bulk ion population with temperature $T_i$. A consequence of the high energy is that the collision frequency between the particles becomes small compared to their transit time around the tokamak [18].

Because of the low collision frequency, the confinement of the fast ions is qualitatively different from that of the thermal bulk ions. The bulk ions are collisionally tightly coupled, typically resulting in significant transport due to turbulent processes. In contrast, the transport of the fast ions is dominated by neoclassical effects, where the width of the orbits of the fast ions becomes the characteristic transport scale.

Charged particles moving in a toroidally axisymmetric tokamak magnetic geometry, in the absence of collisions, follow closed orbits due to the conservation of the constants of motion energy $E$, magnetic moment $\mu = mv_\perp^2/2B$ and canonical toroidal momentum $p_\phi = q\psi - mRv_\phi$ [18]. Here, $m$ and $q$ are the mass and charge of the particle, $v_\phi$ and $v_\perp$ are the toroidal velocity and the velocity component perpendicular to the magnetic field, $R$ is the major radius and $\psi$ is the poloidal magnetic flux.

Due to the non-uniform magnetic field in a tokamak, the ions experience drifts causing them to deviate from the closed magnetic flux surfaces. Additionally, the particles can become trapped on so called banana orbits due to the high gradient of the magnetic field in the toroidal geometry (figure 2.1). This effect prevents them from transiting the inner high-field-side (HFS) and increases the cross-field drifts, resulting in wider orbits.

While fast ion transport is minimal in the axisymmetric case due to the low collisionality, additional magnetic perturbations can result in breaking of the toroidal axisymmetry. This perturbation causes the particle orbits no longer to fully close, resulting in additional drifts, increased fast ion transport and potentially losses of confined ions. Additionally, non-uniform ripple in the toroidal field strength due to the finite number of TF coils can
Fast ions in plasmas

Figure 2.1. Passing and trapped banana orbits overlaid on magnetic flux surfaces in the poloidal cross section.

cause toroidal trapping of the ions, increasing their cross-field drifts by orders of magnitude and causing rapid losses.

2.1 Fast ion sources

Fast ions in fusion plasmas can arise either intrinsically due to processes such as fusion reactions within the plasma, or externally due to injection of fast ions or acceleration in electromagnetic fields. Of particular interest for reactor-relevant plasmas are the fusion-born alpha particles from D-T reactions, as they are responsible for sustaining fusion conditions through self-heating, as well as fast ions produced by auxiliary heating methods. These include neutral beam injection ions, used for initial heating and non-inductive current drive, and ions accelerated by ion cyclotron resonance heating, which uses radio frequency electromagnetic radiation for heating the plasma. This work focuses on neutral beam heating and fusion products, as these are present both on JET and the future reactors.

2.1.1 Neutral beam injection

Neutral beam injection (NBI) is based on the concept of launching high energy neutral atoms into the plasma. These can penetrate deep within the plasma without being affected by the confining magnetic field, before
Fast ions in plasmas

Figure 2.2. Schematic of the NBI operating principle [4].

ionizing in charge exchange (CX) reactions or collisions with the bulk plasma. This allows the ions to deposit heating power throughout the plasma.

A NBI injector consists of a beamline with an ion source, an electrostatic accelerator grid and a neutralizer arranged sequentially (figure 2.2). The ion source creates an initial low temperature plasma, typically either using a heated filament and an arc discharge, or an RF-generated plasma [19]. The ions are extracted using an electrostatic potential and passed into a series of grids forming the accelerator. The grids collimate the ions into a number of beamlets and accelerate them up to 100-1000 keV energy. The high-energy ions then enter the gas-filled neutralizer, where they lose their charge through atomic reactions with the neutral gas, and finally enter the tokamak through a beam duct. Any residual ions are extracted onto an ion dump before entering the tokamak.

The hydrogenic ions generated by the ion source can be either positively or negatively charged. This choice is of particular importance for the neutralizer, where the neutralization efficiency drops dramatically as the energy of the ions increases beyond 100 keV [20]. This is due to the diminishing cross section for the CX reactions, and results in excessive residual ion content, which must be extracted into an ion dump before reaching the tokamak. Negative ions, on the other hand, can efficiently be stripped of the extra electron and neutralized primarily through ion impact processes, which allows for injection of up to 1 MeV neutral beams [21].

As the neutrals enter the plasma, electron and ion impact as well as CX reactions then re-ionize the particles, resulting in a source of fast ions along the neutral beam. As the ions travel through the plasma, they gradually lose their energy in Coulomb collisions with the bulk plasma, depositing energy in the ions and electrons and thus heating up the plasma.
Depending on the toroidal injection angle of the neutral beam, the injected ions can have a substantial fraction of momentum that is parallel to the magnetic field. This momentum is then deposited as torque on the bulk plasma, enabling the beams to increase and maintain the toroidal rotation of the plasma. These ions can also drive a significant toroidal current in the plasma, which can be used for non-inductive operation in tokamaks [22, 23].

### 2.1.2 Fusion products

Fusion products from fusion reactions 1.1-1.3 are another source of fast ions in the plasma. While most of the energy is released in the form of neutrons that escape the plasma upon their generation and do not contribute to plasma heating, a significant fraction is in charged particles that remain confined and can deposit their energy back in the plasma.

The fusion reactions in magnetically confined plasmas can be divided into three categories: thermonuclear, beam-thermal and beam-beam reactions. Thermonuclear fusion takes place between the bulk fuel ions with a reaction rate of

\[
R_{\text{thermal}} = n_{i1} n_{i2} <\sigma v>_{\text{th}}
\]  

where \(n_{i1}\) and \(n_{i2}\) are the densities of the reactant ions and \(<\sigma v>_{\text{th}}\) is the temperature-dependent rate coefficient integrated over the two Maxwellian distributions. The resulting fusion products have correspondingly approximately Maxwellian, isotropic energy distribution peaked around 3.5 MeV [24]. For D-T fusion these reactions are typically dominant, as the bulk ion temperatures can approach the maximum of the D-T cross section (figure 1.1).

Beam-thermal and beam-beam reactions are caused by a beam of fast particles, such as NBI ions or ICRH-accelerated ions, reacting with the thermal plasma and each other with reaction rates of [13]

\[
R_{\text{beam}} = \int \int f_1(\vec{v}_1)\sigma(\vec{v}_1) f_2(\vec{v}_2) |\vec{v}_1 - \vec{v}_2| d\vec{v}_1 d\vec{v}_2
\]  

where \(f_1\) and \(f_2\) are the distribution functions and \(v_1\) and \(v_2\) the velocities of the reactants. For beam-thermal reactions one of the distribution functions is the Maxwellian distribution of the bulk plasma, and can be calculated analytically. Because the energy of the reactants can approach a significant fraction of that of the products, the energy spectrum and distribution of the fusion products can become skewed and broadened [25, 26]. As the D-D fusion cross section peaks around 1 MeV energy, beam-thermal reactions are generally dominant in existing D-D experiments, as the high energy of the beam reactants significantly increases the cross section.

The resulting alpha particles slow down and deposit their energy to the bulk plasma electrons and ions. As the birth energy of the ions is
Fast ions in plasmas

significantly higher than the plasma temperature, the fusion products primarily heat the electron population [18]. For D-D reactions this heating is typically negligible due to the low reaction rates, but the fusion products can be of interest for diagnostic purposes. Since their energies are similar to D-T alpha particles, they can be used as proxies to study reactor-relevant fast ion transport [27].

2.2 Fast ion diagnostics

Measuring properties of fast ions in fusion plasmas is notoriously difficult. As they typically represent a minority population, their fingerprints in any signals are easily masked by those of the bulk plasma. Most techniques involve indirect measurements based on atomic or fusion reactions induced by the fast ions, such as measuring light emitted from CX reactions in fast ion D-alpha diagnostics [5], or measuring the spectra of neutrons and gammas emitted in nuclear reactions with the fast ions [8, 9].

The direct methods include neutral particle analysis (NPA), based on measuring fast ions that neutralize through CX reactions and escape the plasma [28]. The most direct measurements are possible for fast ions escaping the confinement, which can be detected using various fast ion loss detectors [28]. In this work, the focus is on these two key fast ion diagnostics used in the JET tokamak.

2.2.1 Neutral particle analysis

Neutral particle analysis (NPA) is based on measuring the neutral particle flux emitted from the plasma [7]. Fast ions undergoing CX reactions with background atoms lose their charge and can escape the plasma on ballistic trajectories. By determining the energy distribution of these fast neutrals, properties of the original fast ion population can be inferred.

The source of these fast neutrals is the CX reaction rate

\[ S = n_i n_0 <\sigma v>_{CX} \]  

which depends on the fast ion density \( n_i \), background neutral density \( n_0 \), in this work referring to the atomic density, and the CX rate coefficient \(<\sigma v>_{CX}\). The background neutrals can originate from recycling neutrals entering the plasma from the scrape-off layer with energies in the range of 10-100 eV, recombination reactions between plasma ions and electrons with energy equivalent to the plasma temperature, or the neutral beam itself with energies on the order of the fast ions.

The measured fast neutral flux is then the line integral of the source rate
along the diagnostic line of sight

$$\Gamma = \int_0^L S(l)e^{\frac{I_0}{\lambda} - \frac{\lambda}{ds} dl}. \quad (2.4)$$

The exponential term represents the attenuation of the flux due to re-ionization along the path from the source to the detector, primarily resulting from further CX or electron and ion impact reactions with the bulk plasma, with a mean free path of $\lambda$.

As the neutrals enter the diagnostic, they are re-ionized by passing them through a thin stripping foil or a stripping cell filled with neutral gas (figure 2.3). In a conventional $E\parallel B$ NPA layout the ions are then separated using parallel magnetic and electric fields, and their mass and energy can be determined based on their impact location. Particle detectors such as scintillators or solid-state detectors are then used to determine the flux for given energy.

### 2.2.2 Fast ion loss detector

Fast ion loss detectors (FILD) are based on the principle of directly detecting fast ions as they are lost from the plasma. This is particularly useful for the study of processes that enhance fast ion transport and subsequent losses, such as magnetic perturbations and MHD instabilities [29, 30].
Fast ions in plasmas

Loss diagnostics can yield the velocity space distribution of the losses and even quantitatively measure the flux of lost fast ions.

FILD diagnostics are typically located at the end of a probe extending towards the plasma from the vessel walls, where it is exposed to weakly confined fast ions. In some tokamaks, the probe can be maneuvered radially to extend the range of the loss measurements [31].

The detector consists of a scintillator plate registering the strike locations of lost fast ions, and a pinhole collimator to limit the distribution of ions allowed to reach the scintillator (figure 2.4). The gyro motion of the ions in the background magnetic field of the tokamak determines the trajectory and thus the strike location. The energy and pitch angle of the ions can be determined from imaging the light emitted by the plate and mapping the distribution on the plate to the pitch and Larmor radius at the pinhole entrance.

While extremely useful in directly measuring fast ions, FILDs have some significant limitations. The actual distribution function of confined fast ions can only be indirectly inferred from the distribution of losses. The finite extent of the detector also limits the measurable energy and pitch angle to a small part of the velocity space, although multiple or moveable detectors partially alleviate this problem. Finally, the detector cannot be used to distinguish between isotopes, and thus overlapping footprints on the scintillator plate complicate analysis.

Figure 2.4. Operating principle of the FILD diagnostic. Fast ions (blue) following the magnetic field $B$ enter through the aperture (grey) and strike the scintillator plate (red), where the strike point is mapped to the pitch $\xi$ and larmor radius $r_L$ of the ion.
3. Fast ion modelling with ASCOT

Studying the evolution of fast ions with computer models is challenging due to the non-isotropic, non-Maxwellian nature of these particles, which requires kinetic treatment of their full velocity space distribution. This increases the complexity of the problem, as in the most general case their distribution function is 6-dimensional, making direct approaches for solving the distribution function inefficient. Fortunately, thanks to typical low collisionality and minority role of the fast ions, their evolution does not usually need to be solved fully self-consistently. These features enable efficient, Monte Carlo-based methods for solving the distribution function by simulating individual markers in a background plasma, neglecting self-collisions. The primary tool used in this thesis, utilizing this method, is the ASCOT fast particle code [11, 32].

3.1 ASCOT fast ion modelling suite

The Monte Carlo orbit-following code ASCOT solves the distribution function for fast ions in a pre-calculated, fixed toroidal magnetic geometry and background plasma. The evolution of the distribution function $f_s$ for species $s$ is governed by the Fokker-Plank equation

$$\frac{\partial f_s}{\partial t} + \vec{v} \cdot \nabla f_s + \frac{q_s}{m_s} (\vec{E} + \vec{v} \times \vec{B}) \cdot \nabla \vec{v} f_s = C(f_s)$$

(3.1)

where $\vec{x}$, $\vec{v}$ and $t$ are the coordinates corresponding to the position, velocity and time, $q_s$ and $m_s$ are the charge and mass of the species, $\vec{E}$ is the electric field and $\vec{B}$ is the magnetic field. $C(f_s)$ is a collision operator representing interactions with the plasma species, which can be described as convection and stochastic diffusion in the velocity space. This equation can be solved using the Monte Carlo method of averaging over an ensemble of realisations of the stochastic process [33]. In ASCOT this averaging is done by following a marker ensemble representing a minority population and collecting their phase space coordinates in a histogram, which yields
an estimate for the statistical average of the distribution of the original particles.

The trajectories of the markers are solved either by following the full gyro motion around magnetic field lines, or by following the gyro-averaged guiding center of the marker. The gyro orbit is solved with fixed timesteps using the Boris leap-frog algorithm [34]. For the guiding center, the equations of motion [11] are solved with adaptive timesteps using the Cash-Karp algorithm [35], where the error is estimated using the difference between the fourth and fifth-order solutions.

For a steady-state distribution function, the markers are simulated from their source location until they reach certain criteria for their end condition. For example, in the case of neutral beam injection (NBI) heating of a tokamak plasma, the orbits of the markers are followed as they slow down. Once the energy of the markers approaches the temperature of the thermal plasma, defined as a multiple of the local temperature, they are considered thermalized and the simulation is terminated. The Coulomb collisions are simulated using the MCCC [36] Coulomb collision operator, which uses the Milstein method for solving the stochastic differential equation for the diffusion in velocity space.

Particle losses are evaluated by checking the intersections between the particle trajectory and a surface representing the first wall of the device. The wall consists either of a 2D poloidal contour of the limiting surfaces, or an arbitrary 3D triangle mesh. The 3D mesh is stored in an octree structure to enable efficient searching of intersecting triangles, while limiting the number of memory accesses.

Fast ion sources are simulated with additional modules based on the ASCOT code. The beamlet-based Monte Carlo code BBNBI [12] calculates the fast ion source due to NBI injection. The code follows beam neutrals into the plasma starting from the injector, defined as beamlets representing the accelerator grid apertures. Particles passing through the plasma unionized are tallied as shinethrough, and the ionized particles are given to ASCOT as input markers. In BBNBI, the ionization probability is calculated using effective beam-stopping coefficients, which take into account the various processes affecting ionization, such as excitation, electron and ion impact ionization and CX reactions, and average these for a Maxwellian plasma at a given temperature and density. BBNBI can use either analytical fits by Suzuki et al. [37] or tabulated data from the ADAS database [38].

The ASCOT fusion source integrator AFSI [13] is used to calculate the fusion product sources. The code includes various models to calculate the fusion source distributions for thermal, beam-thermal and beam-beam reactions. Markers for ASCOT simulations are then sampled and weighted from the distributions. The Bosch-Hale [3] analytical fits are used to evaluate the fusion cross-sections for D-D, D-T and D-$^3$He reactions. For thermal
Fast ion modelling with ASCOT

fusion, an analytic model with a Gaussian energy spectrum [24] is used to calculate the source rate. A semi-analytic model is used for beam-thermal reactions, where the reaction probability is numerically integrated over the velocity space distribution of the reactants, as calculated by ASCOT. For beam-beam reactions, a Monte Carlo approach is used, where reactants are sampled from arbitrary distributions and the resulting product distributions are calculated kinematically.

3.2 Next generation code ASCOT5

Typical applications for ASCOT use complex 3D geometries and large numbers of markers to achieve sufficient statistical precision, increasing the computational requirements. For example, a high-fidelity simulation for ITER with 3D magnetic field perturbations and a detailed wall model may require tens of thousands of CPU hours. Fortunately, the Monte Carlo approach used by ASCOT is an example of an embarrassingly parallel algorithm, where each marker is simulated independently, which significantly simplifies parallelization.

The previous version of the code, ASCOT4, was parallelized using MPI [39], where separate processes are launched on CPUs connected over a network. They communicate using MPI to divide the work between processes and gather the results after simulation. This approach, however, neglects more recent advances in computing technology, such as multithreading [40] and single instruction, multiple data (SIMD) vectorization [41]. In order to take advantage of the latest supercomputing hardware, as well as simplify the development and maintenance, a new version, ASCOT5, was rewritten as part of this thesis work. The development, validation and benchmarking of the code is described in detail in Publication I.

ASCOT5 has been implemented in the C programming language with a combination of OpenMP [42] and MPI features in a hybrid approach. As with ASCOT4, MPI allows the code to distribute the work to multiple network-connected computing nodes. OpenMP, however, increases the parallelisation within each individual node, enabling the code to run on multiple simultaneous instances, called threads, on a single CPU and utilize vectorized operations that allow the CPU to perform arithmetic operations on multiple values with a single instruction, significantly boosting the throughput of the code. Finally, OpenMP is used to access shared memory, which allows each thread on the same node to share the memory. This allows for larger and more detailed input structures and output distributions, whereas in ASCOT4 the memory was divided between the individual processes and thus limited.

In a typical simulation run, ASCOT5 is launched on multiple nodes using MPI, and the markers are distributed evenly between the processes.
Each process then launches a number of worker threads, typically two for each physical CPU core on the node, which execute identical simulation code for evolving the marker positions, evaluating collisions and collecting distributions. Each thread simultaneously loads and processes $N_{\text{SIMD}}$ markers. The data needed for the calculations, such as marker coordinates and magnetic field components are stored in arrays of length $N_{\text{SIMD}}$, and OpenMP SIMD directives, called *pragmas*, are used to instruct the compiler to convert these operations into single vector instruction calls on the CPU.

Normally the same operations are performed on all markers in sequence, enabling efficient vector operations where each marker is evolved in lock-step with the others. When the simulation of a marker is completed, its end state is stored and it is replaced with another from a queue of unsimulated markers, imposing slight overhead on the simulation. Likewise, some sections of the code, such as updating distributions, where multiple markers may need to access the same memory locations, some overhead is introduced by synchronization. OpenMP provides directives that can handle this overhead efficiently.

Fully utilizing the multithreading and vectorization capabilities of modern supercomputer hardware can potentially enable dramatic increase in performance. For example, the Intel Skylake CPU architecture features two threads per CPU core, and up to 8 double precision values can be computed simultaneously with AVX-512 SIMD operations, yielding a factor of $2 \times 8$ theoretical improvement.

In a realistic case, considering the limitations in memory access speed, bottlenecks between threads and the previously mentioned overhead limit the practical speedup. Benchmarks were performed for representative simulations for a JET-like plasma with NBI ions in an axisymmetric magnetic field, and an ITER-like plasma with fusion alphas in a 3D magnetic field. Comparisons between ASCOT4 and ASCOT5 on Skylake hardware have resulted in approximately 4-7 times faster execution (table 3.1). Particularly in the 3D ITER-like test case, with large 3D magnetic field data being accessed from the memory continuously, reduction in performance is to be expected.

<table>
<thead>
<tr>
<th></th>
<th>ASCOT4</th>
<th>ASCOT5</th>
</tr>
</thead>
<tbody>
<tr>
<td>JET-like 2D</td>
<td>0:36:25</td>
<td>0:05:24</td>
</tr>
<tr>
<td>ITER-like 3D</td>
<td>5:34:58</td>
<td>1:17:00</td>
</tr>
</tbody>
</table>

An additional advantage resulting from the rewrite of the code has been an increase in the maintainability and a reduction in the complexity of the code. ASCOT5 has an explicitly modular structure, with clear interfaces between the various components such as magnetic field, orbit
following and diagnostics. New modules such as different magnetic field representations can be easily implemented using the interfaces without significant modifications to other parts of the code.

Major parts of pre- and postprocessing have also been moved in ASCOT5 to easily maintainable external Python tools, which makes manipulating input and output data more efficient and user friendly. This leaves essentially only the performance-critical parts of the simulation in the core C code, which further supports the maintainability of the code.
4. Validation in JET using synthetic diagnostics

Since detailed simulations of fast ion behavior are ultimately crucial for predictions towards reactor operations, the models used must be validated in existing devices in conditions approaching those in reactors. One method for validation is the use of synthetic diagnostics, which mimic the signal that is expected from diagnostics in an experimental machine based on predicted operating scenarios. Forward modelling involves simulating a case with input parameters close to those in the experimental discharge, calculating the synthetic signal and comparing it to experimental measurements during the discharge. This is used to assess the reliability of predictions and infer possible sources of differences to further refine the models.

For this thesis, the NPA and FILD diagnostics in the JET tokamak were used to validate ASCOT simulations for NBI ions and D-D fusion products.

4.1 Synthetic NPA simulations for NBI ions

An extensive hydrogen campaign was undertaken at JET in 2016 to investigate various isotope effects in pure hydrogen and mixed hydrogen-deuterium plasmas [43]. For a part of the campaign, one of the two NBI injectors was configured to inject hydrogen, while the other was injecting deuterium. This provided the unique opportunity of measuring both fast ion species and validating the ASCOT model for NBI slowing-down using NPA. These results are further discussed in Publication II.

The JET tokamak is equipped with a low-energy neutral particle analyzer which can simultaneously measure the neutral fluxes from hydrogen, deuterium and tritium for energies between 4-97 keV, 5-41 keV and 5-22 keV, respectively. This makes it useful for determining the isotope fraction from the relative fluxes, as well as for diagnosing the NBI ions that were injected at 80 keV for hydrogen and 120 keV for deuterium. The NPA has a radial line of sight along the plasma midplane (figure 1 in Publication II). The line of sight intersects one of the neutral beam
injector trajectories, but only on the high field side of the plasma where the contribution from CX with beam neutrals is negligible.

The fast ion slowing-down distributions were simulated using the ASCOT code, while the beam ionization code BBNBI was used to produce the NBI source. BBNBI follows an injected neutral from the accelerator into the plasma and integrates the ionization probability along the trajectory. When the probability reaches a randomly predetermined value, a fast ion marker representing the injected particles is generated. The generated ensemble was then used in ASCOT to simulate the slowing-down distribution functions for the NBI ions.

To simulate the NPA signal produced by the population, a synthetic diagnostic, based on an earlier version used for ASDEX Upgrade [16], was implemented for the JET NPA geometry. It calculates the line-integrated neutral flux

$$\Gamma = \int_0^L n_i n_0 \langle \sigma v \rangle_{CX} e^{-\int_0^l \frac{n_e \langle \sigma v \rangle_{ion}}{v} dl'} dl$$

(4.1)

The first terms in the integral represents the neutral source from CX reactions with cross section $\langle \sigma v \rangle_{CX}$ between the fast ion population of density $n_i$ and neutral background of density $n_0$. The exponential term represents attenuation due to reionization with cross section $\langle \sigma v \rangle_{ion}$ along the trajectory $l$ from the source to the detector.

The integral is evaluated using the Monte Carlo method of randomly sampling test particles within the viewing cone of the diagnostic, weighted by the local CX reaction rate, and integrating the attenuation along the trajectory towards the NPA entrance. To improve efficiency and avoid following particles that cannot reach the detector, only the contribution from the part of the phase space visible to the detector is used when calculating the source rate.

The background neutral densities were calculated using the FRANTIC code [44] in the JINTRAC integrated modelling suite [45]. A set of 1D neutral density profiles were precalculated for typical densities and temperatures in the hydrogen campaign. This enables fast analysis of a large number of discharges and time slices by selecting a representative neutral density profile parametrized by the central electron density and temperature, without repeating the JINTRAC simulations individually. Representative kinetic profiles for the neutral density calculations were obtained from the JETPEAK database, which contains thousands of samples from steady-state phases of JET discharges.

The synthetic diagnostic workflow was applied to 15 mixed-isotope, mixed-NBI discharges, with the bulk isotope fraction ranging from 10-80% and the NBI power fraction between H and D beams varying between 20-80%. The synthetic signals were fitted to the experimental measurements by scaling the calculated neutral density profiles by up to 65% to account for the uncertainty in the total background neutral level. Impor-
Validation in JET using synthetic diagnostics

Figure 4.1. Measured and synthetic NPA fluxes for two cases with good agreement (top) and poor agreement at low energies (bottom).

...tantly, the same scaling was used for both beam species to maintain the fast ion isotope fraction between the two species.

The synthetic signals were found to qualitatively agree with the experimentally measured neutral fluxes (figure 4.1). The different slowing-down profiles for hydrogen and deuterium were reproduced in most cases, as was the relative fractions of the two isotopes. Some discrepancies were observed at low energies, low power and high concentrations. In these cases the neutral flux from the thermal plasma, which was neglected in these simulations, may be contributing significantly to the measured signal. Also, the results are likely more sensitive to inaccuracies in the neutral density profiles in the low-energy neutral fluxes, as these originate primarily from the pedestal region, where exact details of the recycling and profile shapes are significant.

4.2 Synthetic FILD simulations for fusion products

MeV-range fusion products are routinely measured using the FILD-type lost alpha scintillator probe diagnostic at JET [46]. Measurements of fast ion losses provide an opportunity for validating the ASCOT code and its fusion source model in high performance discharges. These results are discussed in more detail in Publication III.

The scintillator probe at JET measures lost fast ions at energies up to...
Validation in JET using synthetic diagnostics

Figure 4.2. ASCOT 3D model for the scintillator probe and the first wall, with the surface used to tally losses highlighted in red.

1.4 MeV for tritons and 4 MeV for protons, which covers the birth energies of D-D-fusion-born tritons and protons. The fixed probe is located on the low field side midplane, slightly outboard of the poloidal limiters. Because of the limiter shadowing, only prompt losses around the birth energies are typically observed for fusion products.

To accurately model fast ion losses into the probe with ASCOT, a detailed CAD-based 3D wall model of the probe and first wall components were implemented. The model was slightly simplified by removing components not exposed to the fast ions, but all the limiting surfaces retain the full details of the original model. Due to the efficient tree-based wall collision evaluation in ASCOT, nearly the full wall model composed of millions of triangles was used.

While the actual entrance slit on the probe is only 1.2 mm$^2$, an area approximately 2 cm x 5 cm surrounding the entrance on the probe head was used in the model as the surface on which losses are tallied (figure 4.2). This was done to artificially improve the detection efficiency, as even with this large area only approximately 1 in 10 000 markers reaches the probe. The pitch angle and the energy of the losses are recorded, and their distribution is finally mapped onto the scintillator probe using a strike map grid calculated by the Efipdesign tool [46].

The fusion products for the simulations were produced with the ASCOT fusion source integrator AFSI [13]. First, an NBI slowing-down simulation with $10^5$ markers was performed with ASCOT and BBNBI to calculate the fast deuterium distribution. This was then used in AFSI, together with the kinetic profiles of the background plasma, to generate $400 \times 10^6$ markers representing the thermonuclear, beam-thermal and beam-beam protons and tritons, as well as to calculate the D-D neutron rate. The markers were then followed with ASCOT for $5 \times 10^{-4}$ s, sufficiently long for the orbit losses to reach the probe.
Figure 4.3. Poloidal location of the FILD probe in the JET tokamak with flux surfaces in JET discharge #77877.

Figure 4.4. Measured and simulated neutron rates and fast ion losses in the JET discharge #77877.
The discharge used for the validation was an NBI-heated advanced-tokamak-type discharge #77877 with a toroidal field of 2.7 T and a plasma current of 1.8 MA. Simulations were performed for three time slices with varying NBI power. The total neutron rate was in agreement with the measured rate from the fission chamber neutron yield monitors (figure 4.4). While the scintillator probe was not absolutely calibrated, the relative changes in loss rates between the three time slices were likewise found to be within 5-25% with the simulated rates, verifying the AFSI fusion source calculations. The reduction in losses between the first two time slices, despite the constant NBI power, is due to lower density and temperature in the second phase of the discharge.

The phase space distribution of the simulated losses was within 5-10% of the experimentally observed pitch angle and gyroradius extents of the losses (figure 4.5), which was observed around a gyroradius of 11 cm (1 MeV for tritons and 3 MeV for protons) and a pitch angle of 60 degrees. Some likely artificial fringes were observed in the shape of the synthetic losses projected to the scintillator plate. These are likely due to the extended collection area compared to the actual diagnostic. Some of the broadening in the measured losses on the scintillator could also be attributed to the optics and image processing of the signal.
5. Fast ion confinement in ITER and DEMO

5.1 Fast ion losses in ITER due to ELM control coils

ITER will be the first tokamak with a significant population of fast alpha particles from D-T fusion reactions. While earlier experiments at TFTR [47] and JET [48] have measured the effect of alpha particles at small quantities, the baseline ITER operating scenario is aiming for a fusion gain $Q = \frac{P_{\text{fus}}}{P_{\text{aux}}} = 10$. Since alpha particles carry 1/5 of the power produced in D-T reactions, the plasma heating should be dominated by alpha particles.

In order to be able to reach this goal, ITER is combining a number of reactor-relevant systems at a scale larger than previous experiments. One of these is the application of ELM control coils (ECC) (figure 5.1) to mitigate and control edge localized modes (ELM), instabilities occurring at the edge of the plasma in high-confinement-mode operation [49]. These have the potential of ejecting large amounts of energy into the plasma-facing components, and their mitigation is critical for the lifetime of these components [50, 51]. ECCs introduce resonant magnetic perturbations (RMP) which have the effect of reducing the pressure gradients at the plasma edge and thus reducing the magnitude of the instabilities [52].

While beneficial for ELM mitigation, these RMPs also reduce the confinement of fast ions, including fusion alpha particles and NBI ions. This due to the overlapping magnetic islands induced by the perturbations, which enable rapid stochastic transport through the perturbed region. This is demonstrated in a Poincare plot (figure 5.2, top) showing the magnetic field line structure, where the well defined field lines are broken into overlapping stochastic region at $\rho > 0.9$.

The fast ion confinement with RMPs has previously been studied in the vacuum approximation, neglecting the response of the plasma to the perturbations [53, 54, 55, 56]. However, these perturbations induce currents in the plasma that have the effect of reducing the penetration of the perturba-
tions [57]. In the previous studies, the response has been assumed to have a beneficial effect, reducing the losses that otherwise could be increased up to 10-25%. However, detailed modelling with the resistive MHD code MARS-F [58] revealed that, while plasma response indeed restored the field line structure deeper in the plasma, it could increase the stochasticity at the edge, resulting in rapid loss of field lines and confinement. This is depicted in Poincaré plots of the field structure (figure 5.2, bottom), in which the overlapping field lines without plasma response are reorganized and separated, but the edge field lines are lost.

To study the effect of the perturbations and the plasma response on fast ions, ASCOT simulations were performed for fusion alpha particles and 1 MeV NBI ions in the 15 MA ITER baseline scenario (figure 5.3). The Alpha particle and NBI ion birth profiles (figure 5.4) were calculated with the AFSI and BBNBI codes, respectively. While the alpha particles are born throughout the plasma, a significant fraction of the NBI ions are ionized close to the last closed flux surface due to the steep density pedestal in the baseline scenario.

The realistic 3D magnetic field used in the simulations included the toroidal field (TF) ripple due to the 18 TF coils as well as the perturbations due to ferritic components, including ripple-mitigating ferritic inserts and tritium-breeding test blanket modules, the effect of which was modelled using the finite-element solver COMSOL [59]. The vacuum RMP field due to the ECCs was calculated with the Biot-Savart integrator BioSaw [55] using a detailed coil geometry. The coil currents and phasings between the upper, equatorial and lower coil rows were adapted from reference cases based on earlier DIII-D experiments, extrapolated to ITER [60]. Finally, the plasma response due to the RMPs from MARS-F was included by replacing the
Figure 5.2. Poincaré plots of the magnetic field line structure at the plasma edge without (top) and with plasma response (bottom). Each color depicts a separate field line.

Figure 5.3. Electron and ion density and temperature profiles used in the simulations for the ITER 15 MA baseline scenario [59].
toroidal modes $n < 6$ of the vacuum field with the corresponding plasma response modes. The effect in higher modes was found to be negligible.

Without ECCs, both fusion alphas and NBI ions were found to be well confined (table 5.1). Introducing the ECCs with the vacuum approximation dramatically increased the losses, in line with previous studies [53]. The increase in losses is primarily in diffusive losses into the divertor, as the stochasticity depletes the ions born close to the last closed flux surface.

Including the plasma response reduced the losses for fusion alphas as the closed field lines are reintroduced deeper in the plasma where the alphas are born in substantial numbers. However, the losses for NBI ions born near the separatrix are increased by approximately 10%. These losses corresponds to the increased stochasticity in the region $\rho > 0.95$. Including the plasma response was also found to shift the distribution of losses across the divertor, with increased losses seen on the divertor dome (figure 5.5). This was found to be due to the stochastic drift of the turning points on the banana orbits, increasing their diffusion and causing faster losses and
Higher heat loads on the dome.

The power losses due to the ECCs, including plasma response, are approximately 2% for the alpha particles and 3-4% for the NBI ions. The resulting loads on the wall in both cases were approximately 1 MW/m$^2$, which is not a significant concern for the divertor limits. However, an increase in losses underneath the dome was observed due to a secondary turning point inside the divertor for the trapped ions. This has the potential of causing additional heating on the unprotected structures on the underside of the divertor dome. More details on the ITER simulation are presented in Publication IV.

5.2 NBI ion confinement in DEMO under various perturbations

DEMO is the European design for a demonstration fusion power plant as a successor to ITER. Its purpose is to demonstrate the feasibility of production of electricity with fusion, integrating technologies not only for plasma physics, but also for regular operation and maintainability [62, 63]. This implies significantly stricter engineering constraints for various reactor components. One of these is the plasma-facing first wall, for which the designed peak power load should not exceed 1 MW/m$^2$. In addition to the thermal particle and radiative heat fluxes, this also includes fast ion loads, which already for ITER have been previously estimated to reach values greater than 100 kW/m$^2$ [64]. Thus detailed modelling of the predicted fast ion losses is critical for the design process. The modelling presented in this chapter is discussed in more detail in Publication V.

Similarly to the ITER studies, the ASCOT and BBNBI codes were used to model NBI ion losses and wall loads in the European DEMO in a realistic geometry, including perturbations due to TF ripple and ferritic inserts as calculated with BioSaw and COMSOL, respectively. Various magnetic geometries were modelled, including designs with the baseline 18 TF coils as well as 16 coils, and scaling the ferritic insert mass between 25-100% of the reference design. The NBI source model is based on the conceptual
DEMO injector with a power of 16.8 MW and an injection energy of 800 keV.

Like in the ITER case, a significant fraction of the NBI ions were born near the last closed flux surface (figure 5.7) due to the steep pedestal in electron density (figure 5.6). In preliminary simulations losses were observed only for ions born outside $\rho > 0.6$. To speed up simulations, only markers outside this radius were included in the large wall load simulations with a detailed 3D wall (figure 5.7).

The NBI ion confinement was excellent in all cases, with losses remaining below 0.3% even with unmitigated ripple with 18 TF coils (table 5.2). The ferritic inserts further reduced these nearly to the level of unperturbed axisymmetric field, and already at 25% mass reduced the losses by half. Simulations with 16 TF coils increased the losses only up to 2.3%, suggesting this option could be a feasible design from the fast ion point of view. The peak wall loads remained below 40 kW/m$^2$ in all cases (figure 5.8).

The losses were primarily diffusive losses for already slowed-down ions, as the favourable co-current injection geometry minimized orbit losses. The losses on the low field side wall were due to particles with pitch around $\xi = -0.2$, corresponding to deeply trapped banana orbits with
Table 5.2. NBI ion losses in the different magnetic configurations.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>NBI losses</th>
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</thead>
<tbody>
<tr>
<td>Unmitigated Ripple 16 coils</td>
<td>609 kW</td>
</tr>
<tr>
<td>Unmitigated ripple 18 coils</td>
<td>49 kW</td>
</tr>
<tr>
<td>Ripple + 25% FI mass</td>
<td>19 kW</td>
</tr>
<tr>
<td>Ripple + 50% FI mass</td>
<td>8 kW</td>
</tr>
<tr>
<td>Ripple + 75% FI mass</td>
<td>3 kW</td>
</tr>
<tr>
<td>Ripple + ferritic inserts</td>
<td>1 kW</td>
</tr>
<tr>
<td>2D equilibrium</td>
<td>&lt; 1 kW</td>
</tr>
</tbody>
</table>

ripple-enhanced diffusive losses. Some particle losses below the midplane with $\xi \approx 0$ were due to local ripple well trapping, but these had already slowed down to energies below 400 keV before becoming trapped.

In earlier ITER simulations, the shape of the first wall and the gap between the wall and the last closed flux surface (LCFS) has been identified as a key feature in determining the fast ion losses and wall loads [64]. This is both due to the localized losses due to the TF ripple perturbations and details of the tiles comprising the first wall, and it can lead to increased wall loads in hot spots on the tiles. The effect of the first wall shape was studied by varying the distance between the last closed flux surface and the wall between the reference value of 25 cm down to 10 cm (figure 5.9). While the losses increased by 50% at the closest distance, beyond 15-20 cm the losses saturated to a value close to the reference case, suggesting a slightly smaller gap could be feasible, resulting in a slightly more compact and economical design.

Finally, the effect of the scrape-off layer (SOL) density on NBI ionization was studied. Because of the high pedestal density of the reference scenario, and ELMs [65] and SOL blob fluctuations [66], the density outside the LCFS is non-negligible, resulting in ionization of NBI particles before they reach the core plasma. These ions would be rapidly lost, with localized wall loads near the injection port caused by the finite Larmor radius of the ions. This was simulated by artificially increasing the width of the SOL profiles (figure 5.10) using exponential decay in density and temperature. The losses increased significantly as the decay length increased beyond 40-50 mm, producing a stripe of losses originating from the NBI port (figure 5.10). However, such high SOL densities are likely unrealistic in the DEMO operating scenarios.
Figure 5.8. Wall power loads due to NBI ions mapped into a single 20° sector.

Figure 5.9. NBI losses as a function of the distance between the LCFS and the wall at outer midplane.
Figure 5.10. Extrapolated SOL profiles for exponential density decay lengths between 16-77 mm.

Figure 5.11. Particles ionized in the scrape-off layer and losses with increasing SOL density decay length.
6. Conclusion

This dissertation has addressed the issues of predicting energetic particle confinement and losses due to magnetic perturbations in next generation fusion experiments ITER and DEMO using ASCOT fast ion simulations.

For ITER, simulations with ELM control coil induced RMPs showed that including the response of the plasma to the external perturbations is vital, as the response not only affected the magnitude but also the distribution of fast ion losses. The plasma response shifted the fast ion wall and divertor loads, possibly exposing unprotected components to higher fast ion heating. In the case of the ITER baseline operating scenario, however, both alpha particle and NBI losses remained acceptable and compatible with the required ECC fields.

In the case of DEMO, the design was found to be robust with respect to fast ion confinement due to the favourable coil and wall geometry. The sensitivity of fast ion losses due to various magnetic perturbations was studied, including the effects of toroidal field ripple and ferritic inserts in various configurations, together with varying plasma-wall gaps and scrape-off layer conditions. The fast ion losses were found to be acceptable even with the number of TF coils reduced from 18 to 16, which would reduce costs and complexity of the reactor.

For validating the predictions, the ASCOT code was benchmarked with measurements from recent experimental campaigns in 2009 and 2016 in the JET tokamak. A synthetic neutral particle analyser was implemented and applied to NBI simulations in mixed hydrogen-deuterium plasmas. The simulation results qualitatively reproduced the experimentally measured trends in fast neutral fluxes, including the different slowing-down distributions for the fast hydrogen and deuterium ions, as well as the isotope fractions for the two beam species.

A synthetic FILD diagnostic was implemented for the JET lost alpha scintillator probe. This was used to simulate fusion products in high-performance discharges, and the energy and pitch angles of the simulated D-D fusion product losses were within 10% of the measurements, corre-
sponding to prompt proton and triton losses at energies of 3 MeV and 1 MeV, respectively. Additionally, simulations for multiple time slices, with different beam power and plasma parameters, reproduced the time evolution of the measured fast ion losses within 5-10%.

Over the course of the thesis work, a new, highly parallelized version of the ASCOT Monte Carlo code was developed. The new version ASCOT5 substantially increased the performance on modern supercomputer hardware due to OpenMP multithreading and vectorization support, while the complete rewrite of the code simplified its structure, improving its maintainability and extensibility.

The modelling results for the ITER and DEMO studies presented in this dissertation have helped to validate the ITER and DEMO designs, while the JET synthetic diagnostic results support this activity by further validating the ASCOT fast ion models. The tools and methods developed during the work provide a foundation for extending both the validation in upcoming experiments and the predictions for future devices, and the ASCOT5 code has since been used for fast ion modelling in most major tokamaks. Future work will involve applying the tools for new tokamak experiments, including the D-T campaign at JET, and continuing development of ASCOT5 to enable modeling of additional fast ion physics and phenomena.
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References


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