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Divertor conditions in non-linear MHD ELM simulations

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Divertor Conditions in Non-Linear MHD ELM Simulations: Final Report

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Abstract

The world is faced with huge challenges in creating sustainable and clean energy sources. One of the serious candidates to guarantee sufficient clean energy sources is the creation of a nuclear fusion reactor. Presently a world-wide collaboration is building the ITER test reactor in Cadarache. This reactor will demonstrate tenfold power multiplication in a Tokamak in divertor geometry and must deliver a well-established operational scenario. Many of the outstanding issues for the viability of such a reactor have been solved, but there are still several of them remaining. One of those is the understanding and controlling of Edge Localized Modes (ELMs). ELMs are periodic Magneto-Hydro-Dynamic (MHD) instabilities in the edge of the hot plasma destabilized by the pressure gradient in the H-mode edge pedestal. The ELMs lead to high energy loads (up to 10% of total plasma energy in several 100ms) on the wall of the reactor, in particular the exhaust chamber, the divertor. The ability to exhaust or control these power loads is one of the biggest challenges in the development of a commercial fusion reactor.

Some of the physics elements can be extrapolated qualitatively from present day experiments, though more complicated matters, such as the exact energy loads of an Edge Localized Mode, can only be predicted by validated codes. When sufficiently accurate validated codes are developed predictions for ITER as well as commercial fusion reactors can be made. Currently the physics of Edge Localized Modes is not yet well understood. A project called ASTER to simulate a complete cycle of the ELM instability, from its onset to the highly non-linear phase and its decay has been initiated. The non-linear resistive MHD code JOREK is being developed to aid in that objective. One of the issues to be addressed in the development of this code is an improvement in modelling the divertor region and as a first attempt this project has been concerned with the implementation of a simple form of an atomic neutral fluid model in JOREK, where plasma particles that leave the plasma are reflected as cold atomic neutrals. The neutrals are transported diffusively through the plasma where the random walk step size is determined by charge exchange and ionisation and the temperature of the neutrals is to be taken equal to the ion temperature due to strong charge exchange. Ionisation of neutrals (as well as the associated energy losses), depending on the neutral plasma density, the plasma density and the ionisation rate coefficient (and thus the temperature) is taken into account.

JOREK is able to simulate fusion plasmas in circular/limiter geometry as well as x-point/divertor geometry. Since plasma particles leaving the plasma are reflected as atomic neutrals particle conservation is a simple test that needs to be satisfied in order to verify correct implementation of the reflective boundary condition. In circular geometry this condition is well satisfied and the total amount of particles is well conserved. In x-point geometry a substantial amount of particles is lost (10%-20% of the outgoing flux, depending on the grid resolution). The cause of the loss of particles has likely been found. In applying a boundary condition in JOREK the boundary condition as well as it’s derivative along the boundary has to be applied at the grid points at the boundary. JOREK linearizes equations and neglects higher order terms. Since higher order terms show up in the derivative of the reflective boundary condition this condition cannot be directly applied. Inclusion of boundary integrals in JOREK (as present in the weak form of equations in the finite element method) or application of a boundary condition in between grid points instead of the derivative of the boundary condition will likely solve this problem.

Another test to verify correct implementation is comparing the neutral penetration depth to theoretical predictions which indeed shows behaviour results to theoretical predictions. The neutral profile in JOREK has a similar shape as a run performed in EDGE2D, but due to the 3 times lower density in the EDGE2D run the e-folding length is approximately 3 times higher. An exact comparison case in equal geometry still has to be performed.

Due to ionisation of neutrals a decline of temperature is expected near the divertor targets. Unfortunately in contrast to the expected decline a rise in temperature is observed. In JOREK linearised
terms are added to a huge solution matrix which is subsequently solved. It has been found that linearised terms of the temperature equation were added to the wrong place in the solution matrix and correction of this mistake will likely result in the expected temperature rise near the divertor targets. To finally validate the code a new test run has to be performed in which these two problems are corrected.

Despite of the two bugs the code turned out to be stable and a successful simulation of a steady-state solution including neutrals has been achieved. This could be used to simulate the first stages of an Edge Localised Mode. Due to explosion of the neutral density solution at the edge of the outer divertor target a full ELM cycle including neutral particles has not yet been simulated. Running simulations in higher resolution and implementing both necessary corrections will likely result in successful simulation of a full ELM-Cycle with neutrals. After this the effects of the neutral fluid model on the fine structure of the temperature and density profile and the Dα-emissivity can be investigated. As a next step in improvement of the divertor region a separate temperature equation with realistic parallel conductivity coefficients (Spitzer-Harm like) can be implemented. These effects have already been implemented in JOREK and can now be integrated with the implementation of the neutral fluid model. This will allow simulation of the so-called conduction limited regime and when effects for impurities are included detached divertor regimes can also be simulated.

Additional applications for the implementation of the neutral fluid model are massive gas injection and pellet injection. Massive gas injection simulations can now be performed with JOREK and a massive gas injection simulation in circular geometry has been conducted resulting in a disruption as also observed in experiments in Tore Supra. First results are extremely encouraging and reproduce the cooling and destabilisation of the tearing-mode MHD instability.
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Chapter 1

Introduction

The world is faced with huge challenges in creating sustainable and clean energy sources. One of the serious candidates to guarantee sufficient clean energy sources is the creation of a nuclear fusion reactor. Presently a world-wide collaboration is building the ITER test reactor in Cadarache. This reactor will demonstrate tenfold power multiplication in a Tokamak in divertor geometry and must deliver a well-established operational scenario. Many of the outstanding issues for the viability of such a reactor have been solved, but there are still several of them remaining. One of those is the understanding and controlling of Edge Localized Modes (ELMs). ELMs are periodic Magneto-Hydro-Dynamic (MHD) instabilities in the edge of the hot plasma destabilized by the pressure gradient in the H-mode edge pedestal. The ELMs lead to high energy loads (up to 10% of total plasma energy in several 100ms) on the wall of the reactor, in particular the exhaust chamber, the divertor. The ability to exhaust or control these power loads is one of the biggest challenges in the development of a commercial fusion reactor.

Some of the physics elements can be extrapolated qualitatively from present day experiments, though more complicated matters, such as the exact energy loads of an Edge Localized Mode, can only be predicted by validated codes. When sufficiently accurate validated codes are developed predictions for ITER as well as commercial fusion reactors can be made. Currently the physics of Edge Localized Modes is not yet well understood. A project called ASTER to simulate a complete cycle of the ELM instability, from its onset to the highly non-linear phase and its decay has been initiated. The non-linear resistive MHD code JOREK [HC06] is currently being developed to aid in that objective. One of the issues to be addressed in the development of this code is the improvement in modelling the plasma edge and divertor region. Many physical effects, such as ionisation, recombination, dissociation of molecules, association of atoms, charge exchange, impurity physics, play an important role here and lead to different kinds of operating regimes depending on the plasma parameters, see Chapter 2 for an overview. This physical understanding forms a basis for implementations to be made in the JOREK code.

In the rest of this chapter a concise introduction to the energy problem and the need for fusion energy is given, followed by a more technical introduction to fusion energy. Magnetohydrodynamics is introduced that forms a basis for the instabilities that are responsible for Edge Localized Modes. This is followed by an explanation of the heat load problem at the divertor targets of ELM’s. One major objective in the fusion research program is an accurate quantitative estimation of the heat loads after an ELM. An outline of JOREK is given that is being developed to eventually make accurate predictions. The chapter is concluded by an introduction to relevant physics in the divertor region and a concise sketch of the improvements in the JOREK code that have been implemented in this research project.
1.1 The Energy Problem

A very good overview of the energy problem and the advantages of nuclear fusion energy are given in the article written by J. Ongena [OVO04]. The world population is growing and will approximately double in the coming 100 years [wor06]. Further, with the industrial development of third world countries and upcoming powers as China and India the energy usage per capita will also at least double. A global shift of consciousness resulting in much less energy usage per capita is possible, but there is no evidence if or when this would happen. Countries like the Netherlands, Germany and Japan having an average climate and a relatively strong economical development are good norms for average energy usage per capita (3-4.5kW) [ear05] if still adjusted for efficiency gains. Within the next 100 years total power generation has to be at least quadrupled [int08]. The concentration of oil in certain areas of the world leads to political tensions and the increasing population growth and energy usage per capita leads to an ever increasing speed of depletion of fossil fuels.

Besides the depletion of reserves the environmental consequences of burning fossil fuels due to the release of CO$_2$ might even be a much more urgent issue. Huge amounts of CO$_2$ are released into the atmosphere yearly and the CO$_2$ concentration has increased tremendously. Technology is being developed to reduce the release of CO$_2$ into the atmosphere, but this will not reduce the present levels. There is still a big debate going on what the effect of the increasing CO$_2$ concentration in the atmosphere will be. As the ecosystem is very complex it is probably buffered against small changes in the CO$_2$ concentration; similar to buffers in chemistry. The question is, however, where the limits of these buffers are and in what direction the ecosystem will evolve once the stability thresholds are crossed. The possibility of a global climatic change due to the emission of greenhouse gases poses dangers which are not well known, but are possibly very large. In this context it is unavoidable to reduce or stop burning fossil fuels and make the complete switch to other energy sources as soon as possible.

However, a quick and drastic change in sources for energy production is very hard to realize in practise. Although renewable energy sources are inexhaustable they have only limited potential, such as low energy density and fluctuations in time which implies the need for storage which reduces the efficiency even more and increases costs. In this context ‘alternative’ energy sources are not truly alternatives for fossil fuels, because they could never replace all the production for modern society and these energy sources would be better be described as ‘complementary’. Only nuclear fission is well enough developed to replace fossil fuels for large scale energy production, but even fission is only short term (50 years which can be stretched to about 3000 years with breeder technology to transform non-fissile elements into fissile elements) and it has a low acceptance level with the general public (safety issues because of possible chain reactions and the production of highly radioactive waste). The volume of the radioactive waste is rather low (28 tons or 4m$^3$ per GWyr of which 27 tons of waste can be reprocessed and reused; this amounts to 1000kg or about 50 liters of waste per year which becomes about 4m$^3$ after packaging; this is in sharp contrast with the enormous amounts of waste produced by energy production with fossil fuels) and when taking extreme safety measures this is, despite the low acceptance level with general public, the only intelligent choice of energy production that can be employed today until a better alternative is far enough developed.

Future energy generation has to be done in a sustainable fashion. Fusion energy is one of the serious candidates. It was calculated by Goldston et al. [GGG] that fusion energy is very attractive if the probability is more than a few percent that fusion will cost less than the best environmentally acceptable alternative for its potential market share. This justifies serious investment in research for fusion energy.
1.2 Fusion Energy

In fusion reactions energy is released when the total mass of the reaction products is less than the sum of the mass of the initial particles where the energy is released as kinetic energy of the reaction products. By far the most promising reaction for commercial fusion energy is the fusion reaction of hydrogen isotopes Deuterium (D) and Tritium (T). A Helium atom with a kinetic energy of 3.5MeV and a free neutron with a kinetic energy of 14.1 MeV are produced in the fusion reaction amounting to a total energy release of 17.6MeV. A total energy of $3.4 \times 10^{11}$J per gram of reactants is released which is approximately 10 million times higher than the energy contained in a gram of gasoline: $4.4 \times 10^{4}$J. It is the least developed of the three (renewable, fission, fusion), but it holds the promise of being a safe, inexhaustable and rather clean energy production method. It could become the best compromise between nature and the energy needs of our civilization. For 1kg of fusion fuel about 10 million kg of coal or 7 million kg of oil are needed.

Presently there exist two approaches to nuclear fusion: inertial confinement and magnetic confinement. The first is based on micro-implosions of small fuel pellets with lasers or particle beams. Confinement of the fuel is based on the inertia of the pellet fuel mass which resists the natural expansion when it is heated to thermonuclear fusion temperature. Magnetic confinement fusion uses magnetic fields to confine the fuel. Huge progress has been made in the development of magnetic confinement fusion energy.

In a fusion plasma energy is continuously leaking out of the system at a rate $P_L$ so that the energy of the plasma has to be sustained by either an external heating source or by energy produced in fusion reactions. The energy confinement time $\tau_E$ is defined as the ratio between the total energy $W$ contained in the system and the rate of energy loss $P_L$: $P_L = \frac{W}{\tau_E}$. As adequate confinement conditions are obtained, a point is reached where all the necessary heating power to sustain the plasma temperature comes from $\alpha$ particles, which is referred to as ignition of the fusion plasma. The condition for ignition can easily be derived by equating the fraction between the total energy of the plasma and the energy confinement time to the alpha heating power [Wes97] and results in

$$nT\tau_E > 3 \cdot 10^{21} \text{m}^{-3}\text{keVs}$$  

(1.1)

where $nT\tau_E$ is called the fusion triple product. Since the start of fusion energy a 10 million fold increase of the fusion triple product $nT\tau_E$ has been made of which a factor 10000 the last 40 years. Peak production values of 16MW have been obtained in JET with output to input power ratio’s $Q$ of more than 0.6. Fuel for fusion reactions is available for millions of years. Also material needed to build and run fusion reactors appears to be sufficient.

1.2.1 Tokamaks

To avoid end losses when confining the plasma cylindrical tubes are bent in a toroidal shape as shown in Figure 1.1.

The principal magnetic field that confines the plasma is the toroidal magnetic field. This field, however, is not enough for complete confinement of the plasma and in order to have an equilibrium to balance the plasma pressure by magnetic forces it is also necessary to have a poloidal magnetic field. The poloidal magnetic field is primarily generated by a current in the toroidal direction and additionally by poloidal magnetic field coils. This results in a helical magnetic field with components in the toroidal and poloidal direction where the toroidal field is about 10 times stronger as the poloidal field. Most of the magnetic field lines do not return to the initial point after a finite number of turns around the torus, but instead fill a closed surface. In this way nested magnetic flux surfaces are formed.

A very important factor in fusion physics is the safety factor $q$, because of the importance it plays in determining stability. As the magnetic field lines follow a helical path a field line starting at some point in the poloidal plane will return to that place after a certain toroidal angle $\Delta\phi$ which
determines the q-value of this field line:

\[ q = \frac{\Delta \phi}{2\pi} \]  

Rational surfaces play an important role. If \( q = \frac{m}{n} \) where \( m \) and \( n \) are integers the field line joins up on itself after \( m \) toroidal rotations and \( n \) poloidal rotations.

### 1.2.2 Confinement

Reactivity in a plasma increases with both temperature and density, making the plasma pressure a very important variable in attaining fusion reactions. The pressure that can be confined is determined by stability limits and technological considerations. The efficiency of confinement is determined by

\[ \beta = \frac{p}{B^2/2\mu_0} \]  

defining the ratio between plasma pressure and magnetic pressure. The exact processes that limit the confinement of the plasma are not yet completely understood. However, certain improvements of confinement, such as with increasing size of the Tokamak, are found experimentally. It is also found that confinement (in terms of energy confinement time) improves with increasing plasma current, but decreases with increasing plasma pressure. The plasma in the tokamak is first heated to a few keV's by the toroidal current that runs through the plasma and additionally to higher temperatures of \( > 10keV \) by particle beams or electromagnetic waves.

Particle densities in a Tokamak are typically anywhere between \( 10^{19}m^3 \) to \( 10^{20}m^3 \), about a factor \( 10^6 \) than particle densities in the atmosphere. Impurities give rise to radiation losses and dilute the fuel. Low background pressures have to be maintained in order to minimize the penetration of impurities from the vacuum vessel into plasma. Two techniques are currently used to separate the plasma from the vacuum vessel. One is a limiter configuration in which an outer boundary of the plasma (the Last Closed Flux Surface, LCFS) is defined by intersection of the magnetic field with a solid surface. The region inside the LCFS is called the confined plasma and the region outside the LCFS the Scrape-Off Layer. In Figure 1.2 a Tokamak in limiter configuration is shown. A second configuration keeps the particles away from the vacuum vessel by means of modification of the magnetic field which produces a magnetic divertor. This configuration will be employed in ITER and is further explained in the next section.
1.2.3 X-point Geometry and Divertors

In a divertor configuration the Last Closed Flux Surface is defined entirely by the magnetic fields and outside the LCFS the plasma flows towards and eventually interacts with divertor targets. A tokamak in divertor configuration is pictured in Figure 1.3.

Due to modification of the magnetic field at a certain point the magnetic field lines cross each other at the so-called 'x-point', which lies on the separatrix separating the confined region from the outer region. The Scrape-Off Layer designates a narrow region (usually a few cms) outside the separatrix. The Scrape-Off Layer can be thought of as the region where the plasma is 'scraped off' the core plasma. In the SOL the magnetic field lines are open and direct the plasma to solid divertor targets. Plasma particles hitting the walls of the vacuum vessel (including the divertor targets) are able to recombine and desorb back into the plasma. The divertor takes care of exhausting heating power (primarily of alpha particles), exhausting the Helium ash (keeping the He concentration in the core plasma below 10% as not to dilute fuel), controlling the plasma density and fusion power, fuelling the plasma, retaining impurity atoms and molecules within the divertor region and retaining neutrals within the divertor region as not to degrade confinement of the core plasma. Energy can be exhausted locally at the divertor targets or can be radiated over the plasma volume due to impurity particles or plasma particles recombining or falling back to lower states.
1.2.4 Particle and Energy Loads at Divertor Targets

In an ignited plasma the power entering the Scrape-Off Layer is determined by the alpha particle fusion power less the amount of power radiated from the core plasma. The width of this layer is determined by the cross-field thermal diffusivity and the energy loss time (characterized by the energy content of the SOL and the heat flux loss at the targets along the magnetic field). With present estimates of $\Xi_\perp \approx 1\text{m}^2\text{s}^{-1}$ the power e-folding length in the Scrape-Off Layer is approximately $3.7\pm1.1\text{mm}$ [FPM+05]. With a toroidal circumference of about 50m and allowing the power to be spread along two limbs of the divertor results in a total power deposition area of $\approx 0.3\text{m}^2$. A reactor generating a total power output of 3GW produces approximately 600MW of alpha power which results in a heat flux density, provided no other loss mechanisms such as radiation are existent, of approximately $1.8\text{GW/m}^2$, far too high for any solid material in steady state operation (a maximum of about 10MW/m² is allowed).

Methods to decrease power loads to the divertor targets are e.g. injecting or managing impurities to account for volumetric energy losses due to radiation or tilting the divertor targets at a certain angle to the magnetic field lines so that the load is spread over a large area. Also particles can be injected perpendicular to the magnetic field lines, so that the particles are deflected and deposited on a broader range. Different kinds of operation regimes, depending on the plasma density, input power and the atomic/molecular decomposition of the plasma, will also lead to different kinds of
methods for energy deposition.

1.2.5 H-Mode Confinement, Edge Transport Barrier

In the ASDEX Tokamak it was discovered that when sufficient heating power was applied to
the plasma a sudden improvement in confinement, from L-mode confinement to H-mode confinement,
took place (approximately doubling the confinement time). This improvement of confinement was
subsequently observed in many Tokamaks and it will be present in the operating scenario for ITER.
The improved confinement is first observed in the edge of the plasma where a rapid increase in
the pressure gradient takes place, mainly due to an increase in edge density resulting in an edge
transport barrier. This increase in edge density penetrates through the rest of the plasma resulting
in an overall increase of density. The exact reason for it is not clear and may be caused by an
implicit presence of a bifurcation in the solution of the basic transport equations at the transition
point from L to H-mode confinement. Another explanation, which is more widely accepted, is that
a change in the flow profile causes a sudden change in stability of the edge plasma. For transition
from L to H-mode to occur the heating power must be above a certain threshold which can be
deduced from an empirical scaling of data from many tokamaks [Wes97]. Due to the improved
confinement a strong decrease in $H_\alpha$ radiation signal is observed which is caused by a decrease of
recycling of plasma particles as neutrals.

In contrast to improved confinement, the H-mode confinement regime also has several disadvantages
such as uncontrolled transition back to L-mode and improved retention of impurities that dilute
the fuel.

1.3 Magnetohydrodynamics

Magnetohydrodynamics (MHD) is the study of the behaviour of an electrically conducting fluid
in the presence of a magnetic field. Electric currents induced in the fluid as a result of its motion
modify the field; at the same time their flow in the magnetic field leads to mechanical forces
which modify the motion. Magnetohydrodynamics is concerned with describing this interaction
between the field and the motion. In MHD, plasmas are regarded as continuous fluids. The
continuum approach of MHD is usually adequate, but care has to be taken in the case the velocity
distribution is not Maxwellian and a more kinetic treatment is necessary. An extensive outline to
MHD is given in chapter 3.

1.3.1 MHD Instabilities and ELMs

The increase of the gradient in pressure and current in the edge of the plasma gives rise to the
crossing of certain MHD stability limits such as the medium-$n$ ballooning modes and internal
kink modes. The kink mode derives its name from the kinking of the magnetic surfaces and the
plasma boundary. The internal kink mode has its resonant surface on $q = 1$ ($m = 1$ and $n = 1$)
and is driven by the radial gradient of the toroidal current and at higher $\beta$ also by the pressure
gradient. The medium-$n$ ballooning modes are localized modes, centered around their resonant
surfaces. The curvature of the magnetic field lines is stabilizing on the inner side of the torus
and destabilizing on the outer side of the torus. At low pressure gradients the average effect is
stabilizing (provided $q > 1$), but at high pressure gradients it is possible for the perturbation to
be concentrated in the region of destabilizing curvature. See [Wes97] for an extensive introduction
on MHD instabilities. The medium-$n$ ballooning modes and internal kink modes are assumed to
be responsible for the occurrence of Edge Localized Modes (ELMs) in the edge plasma. ELMs
are characterized by $D_\alpha$ spikes in the divertor or limiter region caused by a deterioration in con-
finement which enhances recycling. ELM's are accompanoied by both magnetic and kinetic edge
region fluctuations and localized bursts of MHD activity. They play a key role in mediating energy
and particle transport from the edge which essentially allows steady state operation. There are different types of ELM’s; primarily Type I (frequency increases with increasing heating power, occurrence when heating substantially exceeds H-mode power threshold), Type II (strongly shaped plasma’s), Type III (frequency decreases with increasing heating power, occurrence when heating power slightly exceeds H-mode power threshold), Grassy (intermediating between L and H-mode operating regimes) and ICRF (different type of heating) ELM’s. The power $P_{\text{edge}} = P - P_{\text{rad}}$ reaching the plasma is a key factor in determining the ELM type. Various theories are suggested to explain the ELM phenomenology; see Zohm [Zoh96] for a global overview; but a complete theoretically understanding of ELM’s is not yet existent. Empirically ELMs are well characterized and the most common operating mode in Tokamaks is with type I ELM’s. The repetition frequency ranges from $10 - 200$Hz and their duration is about $100\mu$s. The ITER reference mode has transport losses close to the H-mode power threshold where essentially type III ELM activity takes place. Studying ELM physics and understanding the phenomenology will have to result in optimization and control of ELM’s to enhance overall plasma performance. Mainly the non-linear phase of the ELM is not yet fully understood. Open questions as what determines the amplitude of the ELM energy losses, how the plasma can become unstable, how far the plasma can exceed the MHD stability limits, how the relaxation mechanism works and what determines the pressure gradient and current density after an ELM are still open.

1.4 ELM Energy Loads

The most significant concern of Edge Localized Modes is the energy load deposited at the divertor targets after a type I ELM. This can lead to enhanced erosion at the divertor targets and several different extrapolations to ITER suggest a wide range of possibilities, from acceptable loads to unacceptable loads. Investigating type III ELM’s is important for ITER since the energy loss per ELM is typically a factor of five less than for type I ELM’s. The threshold for erosion is calculated approximately to be $\Delta Q/t^{0.5} \leq 40 \text{MJm}^{-2}\text{s}^{-1}$ [LLK+07] where $\Delta Q$ is the target plate energy density due to an individual ELM and $t$ is the time for that energy to be deposited. Because of the large number of ELMs in a single fusion discharge it is vital to keep the ELM energy flux below this level. The energy striking the divertor target is often seen to be deposited in a width or area about 1-3 times of the steady state heat flux between ELMs. Since the width and the shape of the ELM energy is determined by parallel and perpendicular transport the widening or shifting of the ELM profile in certain experiments is very probably due to modification of the magnetic field topology due to the ELM instability. A good understanding of the ELM instability is necessary to scale the profile towards ITER.

1.5 Research Method: Jorek

There is a variety of different codes to simulate behaviour in a fusion plasma. Many of them are specialized towards certain specific purposes, e.g. modelling of the edge plasma (e.g. EDGE2D, UEDGE) or a variety of MHD codes describing relevant MHD effects (e.g. XTOR, NIMROD, M3D (non-linear codes) and ELITE, MISHKA (linear MHD codes)). A fully functional non-linear MHD code with a significant amount of relevant effects for accurate description of the edge is, however, not yet existent. JOREK is currently being developed to bridge this gap. JOREK is designed to handle realistic geometries that take into account both the core plasma and the plasma boundary (SOL, private flux region and divertor region). The goal is to develop the code such that it can operate on the whole spectrum of relevant time scales (from the Alfven time (1µs) to the equilibrium time(1s)). In the current version of JOREK the reduced MHD equations are solved, but for finer comparisons with experiment implementation of the full MHD equations is
necessary, which is currently being performed. JOREK is concerned with the simulation of a full ELM cycle which has not yet been published. One of the issues to be addressed currently in the development of JOREK is improvement in modelling the edge/divertor region. A more detailed introduction to JOREK is given in Chapter 4.

1.6 Physics in divertor region

Several physical processes play an important role in the edge/divertor region. The type of operating regime (see section 2.3) that is entered is mainly dependent on the density and the energy that is being deposited into the divertor region. The plasma flow at the open field lines at the divertor targets is taken to be equal to the sound speed (Bohm Boundary Condition), see Chapter 2 for an explanation. Plasma particles at the boundary are adsorbed and reflected as atomic neutrals or atomic molecules at the walls. Numerous atomic processes as charge exchange, ionisation and recombination take place and the presence of impurities have a large influence on the behaviour of the plasma.

As a first attempt to improve modelling of the divertor region this project has been concerned with the implementation of a simple form of an atomic neutral fluid model in JOREK, where plasma particles that leave the plasma are reflected as cold atomic neutrals. The neutrals are transported diffusively through the plasma where the random walk step size is determined by charge exchange and ionisation and the temperature of the neutrals is to be taken equal to the plasma temperature due to strong charge exchange. Ionisation of neutrals (as well as the associated energy losses), depending on the neutral plasma density, the plasma density and the ionisation rate coefficient (and thus the temperature) is taken into account. In attaining a steady state solution in JOREK a balance is achieved between the recycling and ionisation of neutrals. Chapter 2 and Chapter 5 give a detailed overview of the implementations made in this research project.

1.7 Summarized Problem Definition

With the emergence of Edge Localized Modes high amounts of energy are expelled from the plasma edge. The JOREK simulation package is currently being developed to simulate the relevant phenomena that play a role in the evolution of an Edge Localized Mode. One of the objectives in simulating these phenomena is accurate predictions of the heat loads after an ELM in arbitrary geometry. The development of the JOREK code is in the stage that improvement of modelling the effects in the divertor region becomes interesting. In this project a neutral fluid model is implemented to account for the recycling of plasma particles as neutrals in the divertor region. Expected effects in obtaining a steady state solution is an increase in plasma density towards the divertor targets, a decline in temperature towards the divertor targets and a slight decline in pressure towards the divertor targets. Steady state profiles are expected to give similar results as specialized 2D divertor codes. The effect of the addition of the neutral fluid model on the heat load profile after an Edge Localized Mode will have to be investigated. Additional applications of the new JOREK simulation package with a neutral fluid model implemented can be explored.
Chapter 2

Divertor conditions and Operation Regimes

In magnetic confinement devices the plasma is confined within closed magnetic flux surfaces. As such fields can only be generated within a restricted volume a boundary is determined by the Last Closed Flux Surface (LCFS). When the closed surface is determined entirely by the magnetic fields the plasma flows towards and eventually interacts with a solid surface. This is the basic setup in a tokamak equipped with a divertor, where the solid surface is removed some distance from the LCFS. The density profile in the Scrape-Off Layer is determined by parallel transport along field lines, anomalous transport across field lines, recycling conditions in the divertor, the temperature profile (determining rate coefficients), the fuelling rate and all kinds of different atomic processes (e.g. charge-exchange, recombination, dissociation, association, ionization). The plasma temperature profile in the region outside of the separatrix, the Scrape-Off Layer (SOL), is determined by the competition of rapid heat transport along the field-lines to the divertor plates, the anomalous heat transport across the flux surfaces, resulting in very small radial decay lengths of the order of a few centimeters and other physical processes such as radiation losses or heat exchange with other species (e.g. neutrals). In this chapter a more comprehensive outline of the different operational regimes and the accompanying relevant physical processes are given in order to further improve modelling of the divertor region in the future. A summary is given of what physical effects have been implemented in this research project.

2.1 Relevant physical processes

2.1.1 Fluid approach

In JOREK a fluid approach is employed resulting from the assumption that kinetic effects can be ignored. This is, however, only the case with high collisionality. Care has to be taken here and sometimes kinetical corrections will have to be employed. If a fluid approach can be employed is determined by the Knudsen number, which is a measure for the mean free path of a particle before it collides in comparison to a characteristic length scale (particles travel along magnetic field lines and the length over which they travel before they are in contact between two solid surfaces is determined by $2L$ where $L$ is the connection length), and has to be sufficiently low:

\[ K^p = \frac{\lambda_{\text{mfp}}}{L} \]  

(2.1)
2.1.2 Sheath Edge and Mach 1 Boundary condition

Because of their lower mass electrons precede ions in flowing to the divertor targets. This sets up an electric field which slows the electrons and drags the ions along. A principal electric field is set up in a narrow sheath near the surface of the divertor targets. In the sheath the ion density is significantly higher than the electron density. As derived in [Sta00] at the sheath edge the plasma flow speed is equal to the sound speed:

\[ c_s = \sqrt{\frac{k_B(T_e + T_i)}{m_i}} \]  

(2.2)

This condition is already implemented in JOREK. However, implementation of this boundary condition in numerical simulations can lead to a large unphysical inflow of density and temperature at the target due to the poloidal component of the \( E \times B \) flow due to an MHD instability. To avoid this unphysical flow, a modified Bohm criterion can be applied following [SC95]:

\[ v || \cdot n + v_E \cdot n = \frac{v || \cdot n}{|v||} c_s \]  

(2.3)

where \( c_s \) is the local sound speed and \( v_E = - R \nabla u \times e_\phi \) the \( E \times B \) flow (drift perpendicular to both the magnetic and electric field) ensuring a positive outflow at the target at an 'equivalent' Mach one.

2.1.3 Energy outflux boundary conditions

Due to the sheath potential electrons are decelerated in the sheath and only electrons of high forward going kinetic energy, at least \( eV_{sf} \), will reach the sheath \( (V_{sf} \) denotes the potential drop that spontaneously arises when the plasma is electrically isolated, thus sheath \( (s) \) is floating \( (f) \), from the solid surface \( ) \). This way the sheath acts as a high energy 'filter' for electrons. Electrons are 'cooled' and the electron temperature across the entire scrape-off layer is reduced. The energy lost by the electrons is transferred to the ions that are accelerated across the sheath. Similarly the pre-sheath also acts to transfer a further amount \( |eV_{pre-sheath}| \approx 0.7k_B T_e \) from the electrons to the ions.

Defining the electron sheath heat transmission coefficient \( \gamma_e \) by

\[ q_{se}^e = \gamma_e k_b T_e \Gamma_{se} \]  

(2.4)

where \( q_{se}^e \) is the electron flux at the sheath edge, amounts to an electron heat sheath transmission coefficient of \( \gamma_e \approx 5.5 \).

Detailed analysis of the ion heat sheath transmission coefficient, see [Sta00], gives a transmission coefficient of \( \gamma_i \approx 2 \) amounting to a total sheath transmission coefficient of \( \gamma \approx 7.5 \). For certain scenarios more complete expressions for \( \gamma \) (e.g. in non-ambipolar conditions, \( T_e \neq T_i \), secondary electron emission and electron reflection, ion reflection, deposition of the potential energy of atom-atom recombination and \( e - i \) recombination on the solid surface) might be necessary, see section 25.5 of [Sta00].

2.1.4 Collisional transfer of energy between electrons and ions

Following Wesson [Wes97] the collisional energy transfer gives rise to the following heating of the ions:

\[ Q_i = \frac{3m_e}{m_i} \frac{n}{\tau_e} (T_e - T_i) \]  

(2.5)
and the following heating of the electrons

\[ Q_e = \eta j^2 + \eta j^2 = \frac{0.71}{e} j \cdot \nabla T_e - \frac{3}{2} \frac{1}{|e| \omega e} j \cdot (b \times \nabla T_e) + \frac{3m_e n_i}{m_i} (T_i - T_e) \] (2.6)

The ohmic heating \( \eta j^2 \) appears in the electron equation only because at a collision only a small fraction (\( \approx \frac{m_i}{m_e} \)) of energy is transferred from the electron to the ion and consequently the scattering of the directed relative motion leads to a predominant heating of the electrons.

The collisional energy transfer between ions and electrons reduces temperature differences between ions and electrons. Implementing this process becomes relevant once a separate equation for electron and ion temperatures is implemented in JOREK.

### 2.1.5 Ionisation of neutrals

Neutrals are ionised by electron impact. For Deuterium atoms the ionisation energy is 14.1eV when atoms are ionised from the ground state. This has been implemented during this project. In more advanced models effective ionisation energies can be used taking ionisation, excitation, photon emission and recombination between different levels into account.

A good fit for the ionisation rate [Vor97] is:

\[
< \sigma v >_{\text{ionisation}} = 0.2917 \cdot 10^{-13} \left( \frac{13.6}{T_e} \right)^{0.39} \frac{1}{0.232 + \frac{13.6}{T_e}} \exp \left( - \frac{13.6}{T_e} \right) \frac{m_i^3}{s} \] (2.7)

In Figure 2.1 the ionisation rate for an electron temperature between 1 and 100000eV is shown.

![Figure 2.1: Ionization Rate](image)

Figure 2.1: Ionization Rate. The most important region is the low temperature region, because at high temperatures most particles will already be ionised. As can be seen in the graph in this region a strong dependence on temperature is the case.
2.1.6 Neutral frictional drag

In a low temperature regime near the targets neutrals can cause frictional drag to the plasma flow before they are ionized. To model this effect an equation for momentum exchange between the neutrals and the plasma flow has to be implemented. This is a very important physical effect, since the neutral ‘cushion’ protects the target, increasing particle confinement times and decreasing particle power deposition on the targets which reduces erosion and heating of the target. To enter this regime it is required that most of the generated alpha power is removed by volume power losses, e.g. radiation. This effect still has to be implemented.

2.1.7 Volume recombination

At very low temperatures near the target (\(T < 1\, \text{eV}\)) volume recombination becomes an important effect. In this sense the sink action of the solid target is replaced by a gaseous target. As in the case for neutral frictional drag this physical effect for to be of importance, most of the generated alpha power has to be removed by volumetric losses. With volume recombination photons are emitted and energy is distributed radially over the plasma.

A good fit for the volume recombination rate [HL65] is:

\[
< \sigma \nu >_{\text{rec}} = 0.7 \cdot 10^{-19} \left( \frac{13.6}{T_e(\text{eV})} \right)^{1/2} \frac{\text{m}^3}{\text{s}}
\]  

which is pictured in Figure 2.2.

Figure 2.2: Recombination Rate. The recombination rate is extremely low at high temperatures, but becomes comparable to the ionisation rate at low temperatures (\(T < 5\, \text{eV}\)).

This effect still has to be implemented and becomes important when low temperature regions are explored.
2.1.8 Atomic processes

Several relevant atomic processes play an important role in the plasma boundary. In the plasma boundary there is existence of hydrogenic particles, in their ground state, several excited states and its ionised state. All states can be modelled by a fluid, provided the Knudsen number of collisionality (a measure for the ratio between the free mean paths of collisionality and characteristic length scales) is sufficiently low. Due to atomic reactions and their accompanying rate coefficients an interesting dynamic between the different kinds of fluids is set up. In addition to hydrogenic atoms there are hydrogenic molecules existent in the plasma that can be a.o. dissociated, dissociatively ionised, molecularly ionised or dissociatively recombined. A similar dynamic is set up for impurity particles that are either sputtered from the wall or injected intentionally. Also reabsorption of atomic line radiation may play an important role, especially in detached regimes. In future advancements of JOREK all these processes may be included and extensive research is going on to accurately model these processes [LLK+07]. The most relevant atomic processes can be found in [Jan87], [Jan95] and [Pos95].

Neutral fluid equation

In the present improvements of the divertor model only an atomic neutral fluid equation is included where the atoms move diffusively through the plasma with the random walk step size determined by charge exchange and ionisation. After a certain penetration depth the atomic neutrals are ionised.

Charge Exchange Rate

No simple fit for the charge exchange rate has been found, except for a complicated fit in the AMJUEL database [Rei04]. Numerical data of the charge transfer rate coefficient is found in [CR82]. The data has been fitted with a function of the type \(< \sigma v > = a \cdot (T/b)^d \cdot \exp \left(-\frac{13.64}{T}\right)\) resulting in:

\[ < \sigma v >_{c.x.} = 4.116 \cdot 10^{-14} \cdot \exp \left(-\frac{13.64}{T}\right) \cdot (T/6)^{0.15} \text{ m}^3 \text{ s} \]  

(2.9)

For lower temperatures (1eV-100keV) the data lies within the same order of magnitude of the actual data and the fit is sufficiently accurate for first simulations. The actual data and the fit are shown in Figure 2.3.

2.1.9 Volume power losses due to hydrogenic or impurity radiation

At low temperatures excited or ionised species can fall back to lower or even their ground states under the emission of photons. This way the energy that went into the ionisation or excitation of the species is distributed radially over the plasma. Impurities are either intrinsic due to sputtering of material surfaces (Beryllium or Carbon) or intentionally injected to increases radiation losses (Neon and Argon are often used for this purpose). The ion temperature of the impurities can usually assumed to be equal to that of the hydrogenic species. Impurity radiation losses are the principal means of reducing the power load to the divertor targets, by radially spreading the energy load over a much larger area. Complex balances between species are set up depending on the rate coefficients.
Figure 2.3: Fit of the Charge Exchange Rate. A strong dependence on temperature is observed in the low temperature region. At higher temperatures the dependence on temperature becomes less strong. At high plasma densities, particles do not penetrate far into the plasma and only the low temperature region of the rate exchange is relevant. At low plasma densities neutrals penetrate far into the high temperature region of the plasma and the whole spectrum of the rate coefficient is relevant.
2.1.10 Recycling of plasma particles as neutrals

The pulse length in tokamaks is usually much longer than the particle replacement time and particles are recycled many times during a discharge. When a plasma ion arrives at a solid surface it undergoes a series of elastic and inelastic collisions with the atoms in the solid. It may either be backscattered after one or more collisions or slowed down in the solid and be trapped. The trapped atoms can subsequently reach the plasma again by diffusion towards the edge of the solid surface. The recycling coefficient defines the ratio of incident flux on the solid surface to the flux returning to the plasma. In addition the flux of plasma particles and the associated radiation energy due to recombination may release particles previously absorbed on the surface leading to recycling coefficients that are significantly greater than unity.

The recycling coefficient depends primarily on the ion energy and the ratio of the masses of the surface atom to the incident ion. Values of $R_E$ and $R_P$ can be found in literature [ERJ92]; the mean backscattered energy being typically about 30%-50% of the incident energy. Complex processes in the edge boundary of the plasma influence the desorption of neutrals back into the plasma. As a simplification in this project it has been employed that plasma particles are reflected as cold atomic Deuterium neutrals that transport themselves diffusively through the plasma. In future implementations the energy of the reflected particles may be taken into account and there may be accounted for additional types of fluids, e.g. molecular neutrals ($D_2$). In many practical cases the backscattered particles consist for about 50% of atoms with energy $\leq 5T_e$ and 50% of low-energy molecules.

2.1.11 Electron parallel energy transport

In the collisional regime ($K^p \ll 1$) the parallel transport can be described by the Braginskii equations with a parallel conductivity for the electrons of

$$\kappa_\parallel = 3.16 \frac{\rho T_e \tau_e}{m_e} = 9.48(2\pi)^{\frac{2}{3}} \frac{\epsilon_0^2 m_D^2 T_e^2}{m_e^2 e^4}$$  \hspace{1cm} (2.10)

2.1.12 Cross field particle and heat diffusivities

Where in parallel energy transport the parallel thermal conductivity scales Spitzer-Hrm like with $T^{5/2}$ the diffusion across field lines anomalous. The exact mechanisms of the anomalous losses are determined by turbulent effects and are not yet completely understood. There has to be relied on scaling studies to accurately model this and big databases are being created to assist in this (e.g. ITER Divertor Modelling database and Database Expert Group).

2.1.13 Neutral diffusion

The neutrals move diffusively through the plasma. Due to strong charge exchange the thermal speed of the neutrals is approximately equal to the thermal speed of the ions [GR95].

Calculating

$$\tau = \frac{1}{n(<\sigma v >_{c.e.} + <\sigma v >_{ionisation})}$$  \hspace{1cm} (2.11)

determined by the ionisation and charge exchange rate coefficients. With $\tau$ the random walk step size can be determined:

$$\lambda = v_{th}\tau = \frac{v_{th}m_D}{\rho(<\sigma v >_{c.e.} + <\sigma v >_{ionisation})}$$  \hspace{1cm} (2.12)

Finally the neutral diffusion coefficient results:

$$D_n = \frac{\lambda^2}{\tau} = \frac{v_{th}^2}{\tau} = \frac{N_{d.o.t} k_B T_i}{\rho(<\sigma v >_{c.e.} + <\sigma v >_{ion})}$$  \hspace{1cm} (2.13)
2.2 Summary of implemented physical effects in this project

2.2.1 Ionisation Rate

The ionisation rate for neutrals

\[
<\sigma v>_{\text{ionisation}} = 0.2917 \cdot 10^{-13} \left(\frac{13.6}{T_e}\right)^{0.39} \frac{1}{0.232 + \frac{13.6}{T_e}} \exp\left(-\frac{13.6}{T_e}\right) \frac{m^3}{s}
\]  

(2.14)

has been implemented. The normalised version of this equation is derived in Section 5.1.

2.2.2 Ionisation Particle Source

The ionisation particle source \( S_i(T_e) \) is equal to (for simplicity dividing the real particle source by the plasma density \( \rho \) and neutral density \( \rho_n \))

\[
S_i(T_e) = \frac{<\sigma v>_{\text{ion}}}{\rho_D} \frac{m^3}{kg s} 
\]  

(2.15)

which amounts to

\[
S_i(T_e) = 8.742 \cdot 10^{12} \left(\frac{13.6}{T_e}\right)^{0.39} \frac{1}{0.232 + \frac{13.6}{T_e}} \exp\left(-\frac{13.6}{T_e}\right) \frac{m^3}{kg s}
\]  

(2.16)

The normalised version of this equation as well as its derivative to the normalised temperature is derived in Section 5.2.

2.2.3 Charge Exchange Rate

A formula for the hydrogen charge exchange rate between plasma particles and neutrals has been implemented in Jorek:

\[
<\sigma v>_{c.x} = 4.116 \cdot 10^{-14} \cdot \exp\left(-\frac{13.64^{1.1}}{T}\right) \cdot (T/6)^{0.15} \frac{m^3}{s}
\]  

(2.17)

A normalised version of this equation is derived in 5.3.

2.2.4 Neutral diffusion coefficient

The neutral diffusion coefficient

\[
D_n = \frac{\lambda^2}{\tau} = \nu_{th}\tau = \frac{N_d\lambda k_BT_i}{\rho(<\sigma v>_{c.c} + <\sigma v>_{\text{ion}})}
\]  

(2.18)

with the ionisation and charge exchange rates given by Equation 2.14 and 2.17 has been implemented in Jorek. The normalised version of this expression as well as the derivatives to the normalised density and temperature are derived in Section 5.4.

2.2.5 Ionisation Energy Losses

Per ionisation event an energy of \( \xi = 14.1\text{eV} \) is consumed. The normalised value is derived in Section 5.5.
2.2.6 Reflective Boundary Condition

At the plasma wall, as well as the divertor targets, plasma particles are reflected as cold neutrals. In the current implementation the neutrals have no separate temperature equation. The following boundary condition is implemented at the plasma boundary (separately for the divertor targets and the boundary aligned to the magnetic field lines):

\[
(D_n \nabla \rho_n = \rho \nu + D \nabla \rho) \cdot n
\]  

(2.19)

See Section 5.6 for a detailed overview of this implementation.

2.2.7 Adjustment of the Plasma Fluid Equation

Neutrals being reflected from the plasma boundary and subsequently being ionised result in a source for the plasma density equation given by \( \rho \rho_n S_i(\hat{T}) \) so that the plasma fluid equation (derived in Section 3.1.4) is adjusted to:

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \nu) + \nabla \cdot (D_\perp \nabla \rho + D_\parallel \nabla \rho) + \rho \rho_n S_i(\hat{T}) + S_{\text{plasma,extra}}. 
\]  

(2.20)

A normalised version of this equation in its weak form as well as its method for implementation is described in Section 5.9.

2.2.8 Addition of a neutral fluid equation in the code

An equation for neutral deuterium particles that transport themselves diffusively through the plasma has been implemented in the code:

\[
\frac{\partial \rho_n}{\partial t} = +\nabla \cdot (D_n(\rho, \hat{T}) \nabla \rho_n) - \rho \rho_n S_i(\hat{T}) + S_{\text{neutral,extra}}
\]  

(2.21)

where the neutral diffusion coefficient is given by Equation 2.2.4. A more extensive description of the implementation as well as the normalisation and the weak form is given in Section 5.8.

2.2.9 Adjustment of the plasma temperature equation

The derivation of the plasma temperature equation requires substitution of the plasma fluid equation, so that adjustment of the plasma density equation also involves adjustment of the plasma temperature equation. Further, with the substitution of the plasma density equation particle diffusive terms have been omitted in former versions of Jorek. This has presently been included. Also, due to energy consumed in ionisation events the temperature equation is altered. The adjusted equation is given by:

\[
\rho \frac{\partial \hat{T}}{\partial t} =
-\rho \nu \cdot \nabla \hat{T} - (\gamma - 1) \rho \hat{T} \nabla \cdot \nu - \hat{T} S_{p,\text{extra}} + S_{T,\text{extra}}
- \hat{T} \rho \rho_n S_i(\hat{T}) - \xi \rho \rho_n S_i(\hat{T})
- \hat{T} \nabla \cdot \left( D_\perp \nabla \rho + (D_\parallel - D_\perp) \frac{B \cdot \nabla \rho}{B^2} B \right) + \nabla \cdot \left( \kappa_\perp \nabla \hat{T} + (\kappa_\parallel - \kappa_\perp) \frac{B \cdot \nabla \hat{T}}{B^2} B \right)
\]  

(2.22)

A detailed overview of the implementation of these adjustments as well as its normalised and weak form can be found in Section 5.7.
2.3 Divertor Operation Regimes

Different operating regimes are determined by varying Coulomb collisionality or varying Knudsen number. Experimentally this coincides with varying density at constant input power or varying radiation losses at constant upstream density.

2.3.1 Sheath Limited Regime

At low separatrix density or high temperature and high collisionality the plasma SOL has very high heat conductivity and the temperature ($T_i$ and $T_e$) along the separatrix can be taken constant (due to conversion of thermal energy into kinetic energy there may be a slight temperature drop at the plates). The heat transfer to the plate is limited by the electrostatic plate sheath potential rather than parallel conductivity. The parallel velocity of particles along magnetic field lines at the plates raises to the sound speed.

2.3.2 Conduction limited regime

At increasing midplane density and increasing collisionality the high recycling regime is obtained. The thermal conductivity is lower than in the sheath limited regime and a parallel temperature gradient is formed and the temperature values near the target are much lower than at the midplane. The conductivity coefficients scale Spitzer-Hrm like, i.e. $T_e^{5/2}$. The parallel ion velocity is low $M < 0.1$ and rises near the target to the sound speed. The pressure is still approximately constant resulting in a steep rise of density near the targets. The density at the targets scales approximately with $\rho_n^3$ and the target temperature approximately with $\frac{1}{\rho_n^2}$. This way physical sputtering is significantly reduced and taking radial spreading into account physical sputtering can be reduced even more. However, due to the strong particle flux there is still a large heat load due to the surface recombination term $\Gamma_D E_B$ and further reduction of the heat load requires lower particle flux to the plate.

2.3.3 Detached plasma regime

At increasing upstream densities or lower power deposition into the divertor (e.g. due to radiation) the electron temperature near the plates falls to a few electronvolts increasing recombination moving the ionisation front upstream. This way the neutral density increases near the plates which decreases the plasma particle flux and also results in strong momentum/pressure losses (due to collision with neutrals) and decreased energy fluxes towards the plates. This is the foreseen operating regime in ITER. For simulation of this regime energy losses due to impurity radiation, momentum losses due to neutral friction and recombination will have to be implemented in Jorek. Also in this regime the parallel plasma velocity raises to the sound speed towards the divertor plates.

2.3.4 Regime employed in this project

In this project the operating regime used is a bit in between the sheath limited and conduction limited regime. The parallel conduction coefficient is still assumed to be constant, but there is operated in a regime of high collisionality. In future implementations it will be interesting to combine the neutral fluid implementations with separate equations for ion and electron temperature where the conductivity scales Spitzer-Harm like to operate in a conduction limited regime. When making comparisons with specialized 2D divertor codes, a regime has to be chosen where the collisionality is so high so that a fluid approach is appropriate, but not too high that modelling of the conduction limited regime is necessary.
Magnetohydrodynamics

Magnetohydrodynamics (MHD) is the study of the behaviour of an electrically conducting fluid in the presence of a magnetic field. Electric currents induced in the fluid as a result of its motion modify the field; at the same time their flow in the magnetic field leads to mechanical forces which modify the motion. Magnetohydrodynamics is concerned with describing this interaction between the field and the motion. In MHD, plasmas are regarded as continuous fluids. Kinetic plasma physics, on the other hand, takes account also of effects involving separate particles, such as the acceleration of some of the charged particles to high energies. Thus MHD is more restricted in scope than plasma dynamics; many of the instabilities of plasma dynamics are not met in MHD. However, the continuum approach of MHD is usually adequate, save for rarefied plasmas and rapidly changing fields. Particle effects and non-maxwellian velocity distributions are, therefore, ignored.

3.1 Derivation of Equations

In [Pri83] the ideal MHD equations in the context for astro-physics are derived. This outline is followed, correcting for resistive effects and adapting scaling for tokamaks to justify assumptions. The behaviour is governed by a simplified form of Maxwell’s equations, together with Ohm’s law, a gas law and equations of mass continuity, motion and energy. Relativistic effects are ignored. The vector/tensor identities that are used in the derivation of the MHD equations can be derived by basic vector/tensor calculus.

3.1.1 Maxwell’s Equations

\[ \nabla \times \mathbf{B} = \mu \mathbf{j} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} \]  
(3.1)

\[ \nabla \cdot \mathbf{B} = 0 \]  
(3.2)

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]  
(3.3)

\[ \nabla \cdot \mathbf{E} = \frac{\rho^*}{\epsilon} \]  
(3.4)

where the magnetic field (\( \mathbf{H} \)) and electric displacement (\( \mathbf{D} \)) have been eliminated by using the relations \( \mathbf{H} = \mathbf{B}/\mu \) and \( \mathbf{D} = \epsilon \mathbf{E} \). In these equations \( \mathbf{E} \) is the electric field, \( \rho^* \) the electric charge
density, \( j \) the current density, \( \mu_0 \) the magnetic permeability and \( \epsilon_0 \) the permittivity of free space such that the speed of light in vacuum is

\[
c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \approx 2.998 \cdot 10^8 \text{ms}^{-1}
\]  

(3.5)

\( \mathbf{E} \) is measured in volts per meter (V m\(^{-1}\)), \( \mathbf{B} \) in Teslas (T) or Webers per square meter (Wb m\(^{-2}\)), \( j \) in Ampere per square meter (A m\(^{-2}\)) and \( v \) in ms\(^{-1}\).

The first Maxwell equation shows that either currents or time-varying electric fields may produce magnetic fields, whereas the third and fourth equations imply that either electric charges or time-varying magnetic fields may give rise to electric fields. The second equation assumes that there are no magnetic poles and implies that a magnetic flux tube has a constant strength along its length.

In magnetohydrodynamics non-relativistic flows are assumed

\[
V_0 \ll c
\]  

(3.6)

with \( V_0 = l_0/t_0 \) a characteristic plasma speed and \( l_0 \) and \( t_0 \) a typical length and time.

Assume

\[
\frac{E_0}{l_0} \approx \frac{B_0}{l_0}
\]  

(3.7)

where \( E_0 \) and \( B_0 \) are typical values of \( E \) and \( B \), so that the two sides of Equation 3.3 have the same order of magnitude.

By comparing the sizes of the terms in Equation 3.1 the second term on the right-hand side (the displacement current) has magnitude

\[
\frac{E_0}{c^2 l_0} \approx \frac{B_0 l_0}{c^2 l_0} = \frac{V_0^2 B_0}{c^2 l_0} \approx \frac{V_0^2}{c^2} |\nabla \times \mathbf{B}|
\]  

(3.8)

which by the non-relativistic assumption is much smaller than the left-hand side of Equation 3.1. This implies that the second term on the ride hand side of Equation 3.1 can be neglected and the first Maxwell equation becomes

\[
\nabla \times \mathbf{B} = \mu j
\]  

(3.9)

Taking the divergence of this equation gives

\[
\nabla \cdot j = 0
\]  

(3.10)

which implies that charge does not accumulate and all currents flow in closed circuits. Another interesting consequence is the ratio of electrostatic and magnetic energy density

\[
\frac{\epsilon_0 E_0^2}{B_0^2/\mu_0} \approx \frac{l_0^2}{t_0^2 c^2} = \frac{V_0^2}{c^2}
\]

which shows that the electrostatic energy is negligble to the magnetic energy.

In this approach the plasma is assumed to be electrically neutral (i.e. \( n_+ - n_- \ll n \) where \( n_+ \) and \( n_- \) are the number densities of positive and negative ions per unit volume and \( n \) is the total number density). From Equation 3.4 the magnitude of the charge imbalance is extracted (\( \rho^* = (n_+ - n_-)e \)) as

\[
\rho^* \approx \frac{\epsilon_0 E_0}{l_0}
\]

and after substituting for \( E_0 \) from Equation 3.7 and putting \( t_0 = l_0/V_0 \)

\[
\rho^* \approx \frac{\epsilon_0 V_0 B_0}{l_0}
\]
The condition for charge neutrality becomes this way
\[ \frac{\epsilon_0 V_0 B_0}{e l_0} = 6 \cdot 10^7 \frac{V_0 B_0}{l_0} \ll n \] (3.11)
with \( B_0 \) in Tesla. Taking \( B_0 = 1 \text{T} \), \( l_0 = 50 \text{m} \) and \( V_0 = 10^5 \text{m/s} \) and \( n = 10^{18} \text{/m}^3 \) the charge neutrality condition as well as the non-relativistic condition are well satisfied.

### 3.1.2 Ohm’s Law

Plasma moving at a non-relativistic speed in the presence of a magnetic field is subject to an induced electric field in addition to the electric field (\( E \)) that would act on the plasma at rest. Ohm’s Law asserts the proportionality to the total electric field (in a frame of reference moving with the plasma) and it can be expressed as
\[ j = \sigma (E + u \times B) \] (3.12)
where \( \sigma \) is the electric conductivity measured in Ohm\(^{-1}\)m\(^{-1}\).

### 3.1.3 Induction Equation

Eliminate \( E \) and \( j \) between Equations 3.9, 3.3 and Ohm’s law (Equation 3.12) to obtain
\[ \frac{\partial B}{\partial t} = -\nabla \times \left( u \times B + \frac{j}{\sigma} \right) = \nabla \times \left( u \times B \right) - \nabla \times \left( \eta \nabla \times B \right) \] (3.13)
where \( \eta = 1/\mu \sigma \) is the magnetic diffusivity. With proper normalization (Section 4.4) this can be written as:
\[ \frac{\partial B}{\partial t} = -\nabla \times E = \nabla \times \left( v \times B - \eta J \right) \] (3.14)

### 3.1.4 Mass Continuity

The equation of mass continuity is well known and can be expressed in its differential form as
\[ \frac{D\rho}{Dt} + \rho \nabla \cdot u = 0 \] (3.15)
or
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \] (3.16)
where
\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + u \cdot \nabla \]
The equation implies the increase of density when an inflow of mass is present, whereas it decreases when the plasma diverges out of the region. This equation is valid for both ionized and neutral fluids, so, after adding diffusive effects and source terms (e.g. ionization or recombinatio) two equations can be deduced. In this equation a separate source term for ionization is taken into account:
\[ \frac{\partial \rho_i}{\partial t} = -\nabla \cdot (\rho_i u_i) + \nabla \cdot (D_{i\perp} \nabla \rho_i + D_{i\parallel} \nabla \rho_i) - \frac{\rho_p n}{m_D} < \sigma v >_{\text{ion}} + S_{\text{plasma,extra}} \] (3.17)
\[ \frac{\partial \rho_n}{\partial t} = -\nabla \cdot (\rho_n u_n) + \nabla \cdot (D_n \nabla \rho_n) - \frac{\rho_p n}{m_D} < \sigma v >_{\text{ion}} + S_{\text{neutral,extra}} \] (3.18)
For simplicity it will be assumed that the diffusive term in the neutral density equation dominates the convective term and the neutral density equation can be simplified to:
\[ \frac{\partial \rho_n}{\partial t} = +\nabla \cdot (D_n \nabla \rho_n) - \frac{\rho_p n}{m_D} < \sigma v >_{\text{ion}} + S_{\text{neutral,extra}} \] (3.19)
3.1.5 Newton’s Second Law of Motion

Under conditions of electrical neutrality, the equation of motion may be written

$$\rho \frac{Du}{Dt} = -\nabla p + j \times B + \nu \nabla^2 v$$

(3.20)

where \( \rho \) is the mass density, \( p \) the plasma pressure and the material is, in general, subject to a plasma pressure gradient \( \nabla p \), a Lorentz force \( (j \times B) \) and a viscosity term.

Simple rewriting gives (with \( p = \rho T \) in normalized form as justified further on):

$$\rho \frac{\partial v}{\partial t} = -\rho v \cdot \nabla v - \nabla (\rho T) + B \times J + \nu \nabla^2 v$$

(3.21)

3.1.6 Energy Equation

The evolution of temperature can be deduced from the energy equation:

$$\frac{\partial p}{\partial t} + v \cdot \nabla p + \gamma p \nabla \cdot v = -L$$

(3.22)

where \( L \) is the energy loss function. For the energy loss function thermal conduction, the energy losses due to ionization events and an extra specifiable heat source are considered, so that \( L \) is equal to:

$$L = -\left( \nabla \cdot \{ \kappa_\perp \nabla_\perp T + \kappa_\parallel \nabla_\parallel T \} + S_T \right) + \frac{\xi \rho_p}{m_D} < \sigma v >_{\text{ion}}$$

(3.23)

Substituting \( L \) in Equation 3.22 and substituting \( p = \rho T \) gives

$$\rho \frac{\partial T}{\partial t} =$$

$$-T \frac{\partial \rho}{\partial t} - \rho v \cdot \nabla T - T v \cdot \nabla \rho - \gamma \rho T \nabla \cdot v + \nabla \cdot \left( \kappa_\perp \nabla_\perp T + \kappa_\parallel \nabla_\parallel T \right)$$

$$-\frac{\xi \rho_p}{m_D} < \sigma v >_{\text{ion}} + S_{T, \text{extra}}$$

(3.24)

Now substituting the plasma density equation, Equation 3.17 and working out the perpendicular and parallel gradients of \( \rho \) and \( T \) gives

$$\rho \frac{\partial T}{\partial t} =$$

$$-\rho v \cdot \nabla T - (\gamma - 1)\rho T \nabla \cdot v - TS_{\rho, \text{extra}} + S_{T, \text{extra}}$$

$$-T \frac{\rho_p}{m_D} < \sigma v >_{\text{ion}} - \frac{\xi \rho_p}{m_D} < \sigma v >_{\text{ion}}$$

$$-T \nabla \left( D_\perp \nabla \rho + (D_\parallel - D_\perp) \frac{B \cdot \nabla \rho}{B^2} B \right)$$

$$+ \nabla \left( \kappa_\perp \nabla T + (\kappa_\parallel - \kappa_\perp) \frac{B \cdot \nabla T}{B^2} B \right)$$

(3.25)
There is a variety of different codes to simulate behaviour in a fusion plasma. Many of them are specialized towards certain specific purposes, e.g. modelling of the edge plasma (e.g. EDGE2D, UEDGE), or employ a kinetic/monte carlo approach towards fusion plasma modelling (e.g. Eirene). A fully functional MHD code that can be employed towards a great variety of different MHD effects (e.g. instabilities as tearing modes, internal kink instabilities and edge localized modes), that can work in realistic geometries, that has a significant amount of edge physics included and that can operate on a great variety of different timescales (from the Alfven time ($1\mu$s) to the equilibrium time(1s)) is not yet existent. The non-linear resistive MHD code JOREK is currently being developed to aid in this objective. In the current version of JOREK the reduced MHD equations are solved, but for finer comparisons with experiment implementation of the full MHD equations is necessary, which is currently being performed.

4.1 Jorek Grid

An example of a JOREK grid is given in Figure 4.1. This Figure shows a Tokamak setup in divertor geometry. JOREK is also capable of working with circular geometries. The poloidal geometry is decomposed into $N_E$ quadrilateral cells parameterized with a Bezier approach. The resolution can be adjusted in 5 different directions:

- A: Core plasma in the radial direction.
- B: Core plasma in the poloidal direction.
- C: Direction perpendicular to open field lines.
- D: Resolution perpendicular to the divertor plates.
- E: Resolution in private flux region.

It is possible to have higher resolution at the separatrix and plasma boundary relatively to elements further away from the separatrix/plasma boundary. The divertor geometry in Jorek is very basic and implies a solid boundary at a certain angle to the magnetic field lines. In future versions of Jorek a more complex divertor geometry will have to be implemented.

4.2 Boundary types

Jorek has 3 types of boundaries:
Figure 4.1: Grid in Jorek. The poloidal cross-section is subdivided into finite elements. The resolution can be adjusted in several directions. The resolution towards the separatrix and the plasma boundary can be increased relatively to points further away from the plasma boundary and separatrix.

- **Type 1 boundary**: These grid points lie on one of the divertor targets.

- **Type 2 boundary**: These grid points lie on the boundary that is aligned with a magnetic flux surface. Also grid points on the boundary of the private flux region belong to this type.

- **Type 3 boundary**: Corner points that constitute both types of boundaries.
4.3 Toroidal Coordinate System

A toroidal coordinate system is adapted defined by \((R,Z,\phi)\). The real parameters in the poloidal plane can be mapped on a local isoparametric coordinate system \((s,t,\phi)\) with \(s\), \(t\) the local parameters of a region in the poloidal plane. A co-variant basis can be defined as follows:

\[
\begin{align*}
a_1 &= J(\nabla t \times \nabla \phi) \\
a_2 &= J(\nabla \phi \times \nabla s) \\
a_3 &= J(\nabla s \times \nabla t)
\end{align*}
\]

where

\[
J^{-1} = \nabla s \cdot \nabla t \times \nabla \phi
\] (4.1)

is the Jacobian.

A contravariant basis can be defined as follows:

\[
\begin{align*}
a^1 &= \nabla s \\
a^2 &= \nabla t \\
a^3 &= \nabla \phi
\end{align*}
\]

The vectors are in general not orthogonal:

\[
\begin{align*}
a_i \cdot a_j &= g_{ij} \\
a^i \cdot a^j &= g^{ij} \\
a_i \times a_j &= J\epsilon_{ijk} a^k \\
a^i \times a^j &= \frac{1}{J}\epsilon_{ijk} a_k
\end{align*}
\]

where the metric coefficients are given by:

\[
\begin{align*}
g_{11} &= \frac{J^2}{R^2} |\nabla t|^2 \\
g_{22} &= \frac{J^2}{R^2} |\nabla s|^2 \\
g_{12} = g_{21} &= -\frac{J^2}{R^2} \nabla s \cdot \nabla t \\
g_{33} &= R^2 \\
g^{11} &= |\nabla s|^2 \\
g^{11} &= |\nabla t|^2 \\
g^{12} = g^{21} &= \nabla s \cdot \nabla t \\
g_{33} &= \frac{1}{R^2}
\end{align*}
\]
4.4 Normalisation

The pressure in Jorek is defined by:

\[ p = \rho \hat{T} \]  

(4.2)

where the temperature \( \hat{T} \) is defined in J/kg. The temperature \( T \) in eV is converted to \( \hat{T} \) by the following formula:

\[ \hat{T} = \frac{e}{m_D} T = 4.790 \cdot 10^7 T \]  

(4.3)

All variables in JOREK are normalised using the mass density \( \rho_0 \) at the axis and the magnetic permeability \( \mu_0 \):

- \( \tilde{\rho} = \frac{1}{\rho_0} \rho = 2.994 \cdot 10^{26} \frac{\rho}{\rho_0} \)
- \( \tilde{D} = \sqrt{\mu_0 \rho_0 D} = 6.47 \cdot 10^{-7} \sqrt{\mu_0} D \)
- \( \tilde{\mu} = \sqrt{\frac{\mu_0}{\rho_0}} \mu = 1.93 \cdot 10^{10} \frac{\mu}{\mu_0} \)
- \( \tilde{\eta} = \sqrt{\frac{\mu_0}{\rho_0}} \eta = 5.16 \cdot 10^{-11} \sqrt{\mu_0} \eta \)
- \( \tilde{\kappa} = \sqrt{\frac{\mu_0}{\rho_0}} \kappa = 1.93 \cdot 10^{10} \frac{\kappa}{\mu_0} \)
- \( \tilde{S} = \sqrt{\frac{\mu_0}{\rho_0}} S = 1.93 \cdot 10^{10} \frac{S}{\mu_0} \)
- \( \tilde{S}_i = \sqrt{\mu_0 \rho_0^2} S_i = 2.168 \cdot 10^{-43} \frac{\rho_0^2}{\mu_0} S_i \)
- \( \tilde{S}_T = \sqrt{\rho_0 \mu_0^2} S_T = 8.135 \cdot 10^{-23} \mu_0 S_T \)
- \( \tilde{T} = \mu_0 \rho_0 \tilde{T} = 4.195 \cdot 10^{-33} \mu_0 \tilde{T} \)
- \( \tilde{\rho} = \mu_0 \rho = 1.256 \cdot 10^{-6} \rho, \tilde{J} = \mu_0 J = 1.256 \cdot 10^{-6} J \)
- \( \tilde{E} = \sqrt{\mu_0 \rho_0} E = 6.47 \cdot 10^{-7} \sqrt{\mu_0} E \)

The following transition from the temperature in electronvolts to the normalised Jorek temperature holds:

\[ \hat{T} = e \mu_0 n_0 T \]  

(4.4)

4.5 Finite element method

A finite element method using Bezier patches is applied to the MHD simulations performed in Jorek [CH08]. A major advantage of this strategy is the possibility to implement a flexible mesh refinement strategy. There are 4 degrees of freedom at every node and every variable as well as its derivative is continuous at every grid point. The problem is discretized by finite elements and written in its weak form. All degrees of freedom are assembled into a huge 'stiffness' matrix of order \( 5 \cdot 10^6 \) which has to be solved at every timestep.
4.5.1 Finite Elements

Surfaces in Jorek are represented by Bezier objects which are defined by Bernstein polynomials and accompanying control points [CH08]. At every grid point this amounts to 9 degrees of freedom. Due to requirements of continuity of the surface and continuity of the derivatives in both tangent directions and the cross-derivative this amount is reduced to 4 degrees of freedom, namely the value at the grid point, the derivative in the s-direction, the derivative in the t-direction and the cross-derivative (partial derivative to both s and t).

4.5.2 Representation of variables

Variables in JOREK are represented by finite elements in the poloidal plane and Fourier harmonics in the toroidal direction:

\[
U(s, t, \phi) = \text{Re} \left( \sum_{n=0}^{N_{\text{tor}}-1} \sum_{i=1}^{N_{\text{nodes}}} \sum_{j=1}^{4} u_{ijn} H_j(s, t) e^{in\phi} \right)
\]  

(4.5)

where the variables \( H_j(s, t) \) represent the newly implemented Bezier finite elements.

4.5.3 Time Stepping

To allow for large time steps a fully implicit Crank-Nicholson approach is used in Jorek. The system of equations can be written in the following general form:

\[
\frac{\partial A(\zeta, t)}{\partial t} = B(\zeta, t)
\]  

(4.6)

where \( A \) and \( B \) are sets of independent equations and \( \zeta = (\zeta_i) \) are the physical unknowns. \( A(\zeta, t) \) and \( B(\zeta, t) \) may depend non-linearly on \( \zeta \) and \( t \). Through the Cranck-Nicholson scheme Equation 4.6 becomes:

\[
\delta A^n = \frac{\delta t}{2} [B^{n+1} + B^n]
\]  

(4.7)

where \( \delta t \) is the time step and superscript \( n \) denotes a value at time iteration \( n \). The advantage of this method is that linearization in first order keeps second order accuracy. Rewriting

\[
\frac{\delta t}{2} [B^{n+1} + B^n] = \frac{\delta t}{2} [B^{n+1} - B^n + 2B^n]
\]

and linearizing \( B \) with respect to \( \zeta \):

\[
B^{n+1} - B^n = \left( \frac{\partial B}{\partial \zeta} \right)^n \cdot \delta \zeta^n
\]  

(4.8)

so that Equation 4.7 reduces to

\[
\delta A^n - \frac{1}{2} \delta t \left( \frac{\partial B}{\partial \zeta} \right)^n \cdot \delta \zeta^n = \delta t B^n
\]  

(4.9)
4.6 Reduced MHD Equations

For many physics studies it suffices to express the magnetic field $B$ in terms of a potential $\psi$ and the velocity $v$ in terms of a parallel velocity $v_{\parallel}$ (properly normalised) and a potential $u$ as is done in the following equations, following [BZV98]:

$$B = \frac{F_0}{Re_\phi} + \frac{1}{R} \nabla \psi(t) \times e_\phi$$  \hspace{1cm} (4.10)

$$v = -R \nabla u \times e_\phi + v_{\parallel}B$$  \hspace{1cm} (4.11)

$$J = \Delta^* \psi$$  \hspace{1cm} (4.12)

$$w = \nabla^2_{\perp} u$$  \hspace{1cm} (4.13)

In this way ion density $\rho_i$, neutral density $\rho_n$, temperature $T$, velocity potential $u$, parallel velocity $v_{\parallel}$ can be evolved in time:

$$\frac{\partial \rho_i}{\partial t} = -\nabla \cdot (\rho_i v) + \nabla \cdot \left( D_{\perp} \nabla_{\perp} \rho_i + D_{\parallel} \nabla_{\parallel} \rho_i \right) + S_{\rho_i}$$  \hspace{1cm} (4.14)

$$\frac{\partial \rho_n}{\partial t} = -\nabla \cdot (\rho_n v) + \nabla \cdot \left( D_n \rho_n \right) + S_{\rho_n}$$  \hspace{1cm} (4.15)

$$B \cdot \left( \rho \frac{\partial v}{\partial t} \right) = -\rho v \cdot \nabla v - \nabla (\rho T) + J \times B + \nu \nabla^2 v$$  \hspace{1cm} (4.16)

$$e_\phi \cdot \nabla \times \left( \rho \frac{\partial v}{\partial t} \right) = -\rho v \cdot \nabla v - \nabla (\rho T) + J \times B + \nu \nabla^2 v$$  \hspace{1cm} (4.17)

$$\frac{1}{R^2} \frac{\partial \psi}{\partial t} = +\eta \nabla \cdot \left( \frac{1}{R^2} \nabla_{\perp} \psi \right) - B \cdot \nabla u$$  \hspace{1cm} (4.18)

In JOREK these equations are evolved in time and solved in their weak forms. In the weak form the equation is multiplied by a test function, integrated over the domain and subsequently partially integrated (see Sections 5.7, 5.8 and 5.9 for examples of equations written in their weak forms).
In this chapter the implementations described in Chapter 2 are described in extensive detail. First an expression for the normalised ionisation rate is derived (Section 5.1), followed by an expression for the plasma particle source term that results due to ionisation events (Section 5.2). Thirdly a normalised expression for the charge exchange rate (Section 5.3) is derived which forms a basis for the derivation of the normalised neutral diffusion coefficient (Section 5.4). As fifth a normalised value for the ionisation energy (Section 5.5) is calculated. These expressions form a basis for the implementations to be performed in the implemented reflective boundary condition (Section 5.6) and the weak forms of the plasma fluid equation (Section 5.9), neutral fluid equation (Section 5.8) and temperature equation (Section 5.7). For simplicity reasons the tilde describing normalised values has been omitted in Sections 5.6, 5.7, 5.8 and 5.9. Please note, however, that the implemented variables are nonetheless normalised as described in Section 4.4.

5.1 Normalised ionisation rate

The ionisation rate [Vor97] is given by:

$$<\sigma v>_{\text{ion}} = 0.2917 \cdot 10^{-13} \left(\frac{13.6}{T_e}\right)^{0.39} \frac{1}{0.232 + \frac{13.6}{T_e}} \exp\left(-\frac{13.6}{T_e}\right) \text{m}^3\text{s}^{-1}$$

(5.1)

with $T_e$ in eV.

Using the normalisation conversions as outlined in Section 4.4 the ionisation rate can be written as (taking the electron temperature to be equal to the plasma temperature):

$$<\sigma v>_{\text{ion}} = 0.2917 \cdot 10^{-13} \left(\frac{13.6\mu_0n_0e}{T}\right)^{0.39} \frac{1}{0.232 + \frac{13.6\mu_0n_0e}{T}} \exp\left(-\frac{13.6\mu_0n_0e}{T}\right) \text{m}^3\text{s}^{-1}$$

(5.2)

Defining

$$E = 0.2917 \cdot 10^{-13},$$

(5.3)

$$F = 0.232,$$

(5.4)

and

$$G = 13.6\mu_0en_0 = 2.738 \cdot 10^{-24}n_0$$

(5.5)

gives

$$<\sigma v>_{\text{ion}} = E \left(\frac{G}{T}\right)^{0.39} \frac{1}{F + \frac{G}{T}} \exp\left(-\frac{G}{T}\right)$$

(5.6)
5.2 Normalised ionisation particle source

The ionisation particle source is defined as:

\[ S_i = n_m <\sigma v> \]  

(5.7)

For simplicity reasons the ionisation particle source is redefined here by transforming it to its value expressed in mass density while dividing it by the plasma mass density and the neutral mass density, resulting in:

\[ S_i(T_e) = \frac{<\sigma v>}{m_D} \]  

(5.8)

Taking the electron temperature equal to the plasma temperature with

\[ R = \frac{0.2917 \cdot 10^{-13}}{m_D} = 8.701 \cdot 10^{12} \]  

(5.9)

gives

\[ S_i(T) = R \left( \frac{G}{T} \right)^{0.39} \frac{1}{F + \frac{G}{T}} \exp \left( - \frac{G}{T} \right). \]  

(5.10)

With

\[ \tilde{S}_i = 2.168 \cdot 10^{-43} n_0^{2.0} S_i \]

and

\[ U = 2.168 \cdot 10^{-43} n_0^{2.0} \]  

(5.11)

for the normalised ionisation particle source is found:

\[ \tilde{S}_i(\tilde{T}) = U \cdot R \left( \frac{G}{\tilde{T}} \right)^{0.39} \frac{1}{F + \frac{G}{\tilde{T}}} \exp \left( - \frac{G}{\tilde{T}} \right). \]  

(5.12)

Taking the derivative to \( \tilde{T} \) gives:

\[ \frac{\partial \tilde{S}_i}{\partial \tilde{T}} = \frac{U \cdot R \cdot G}{T^2 (F + \frac{G}{T})} \exp \left( - \frac{G}{T} \right) \left( \frac{G}{T} \right)^{0.39} \left( \frac{1}{F + \frac{G}{T}} + 1 - \frac{0.39G}{G} \right). \]  

(5.13)

5.3 Normalised charge exchange rate

The fit for the charge exchange rate is given by:

\[ <\sigma v >_{c,x} = 4.116 \cdot 10^{-14} \cdot \exp \left( - \frac{13.64^{1.1}}{T} \right) \cdot \left( \frac{T}{6} \right)^{0.15} \]  

(5.14)

Replacing \( T \) with the normalised variable \( \tilde{T} \) gives

\[ <\sigma v >_{c,x} = 4.116 \cdot 10^{-14} \cdot \exp \left( - \frac{17.71 \cdot (\mu_0 n_0 e)^{1.1}}{\tilde{T}} \right) \cdot \left( \frac{\tilde{T}}{6\mu_0 n_0 e} \right)^{0.15} \]  

(5.15)

With

\[ J = 1.593 \cdot 10^{-10} n_0^{-0.15}, \]  

(5.16)

\[ C = 1.209 \cdot 10^{-26} n_0^{1.1}, \]  

(5.17)

this gives

\[ <\sigma v >_{c,x} = J \cdot \exp \left( - \frac{C}{\tilde{T}^{1.1}} \right) \cdot \tilde{T}^{0.15}. \]  

(5.18)
5.4 Normalised Neutral Diffusion Coefficient

The neutral diffusion coefficient is given by:

\[
D_n = \frac{\lambda^2}{\tau} = v_{th}^2 = \frac{N_{d.o.f} k_B T_i}{\rho \langle <\sigma v >_{c.e.} + <\sigma v >_{ion} \rangle} \tag{5.19}
\]

Taking the ion temperature to be equal to the plasma temperature and substituting for the normalised temperature and normalised density gives:

\[
D_n = \frac{N_{d.o.f,mD}}{\mu_0 n_0^\frac{3}{2}} \frac{\tilde{T}}{\tilde{\rho}} \langle <\sigma v >_{c.e.} + <\sigma v >_{ion} \rangle \tag{5.20}
\]

With

\[
A = \frac{N_{d.o.f,mD}}{\mu_0 n_0^\frac{3}{2} m_D^2} = \frac{N_{d.o.f}}{\mu_0 n_0^\frac{3}{2} m_D} = 2.3798 \cdot 10^{12} \frac{N_{d.o.f}}{n_0^3} \tag{5.21}
\]

this gives:

\[
D_n = \frac{A \frac{\tilde{T}}{\tilde{\rho}}}{J} \cdot \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right) \cdot \tilde{T}^{0.15} + \frac{E \left( \frac{G}{T} \right)^{0.20}}{F + \frac{G}{T}} \cdot \exp - \left( \frac{C}{T} \right) \tag{5.22}
\]

Normalising \(D_n\) with

\[
H = \sqrt{\mu_0 \rho_0} = 6.482 \cdot 10^{-17} \sqrt{n_0} \tag{5.23}
\]

gives

\[
\tilde{D}_n = \frac{A \cdot H}{\tilde{\rho}} \cdot \frac{F \tilde{T} + G}{J \cdot \left( F + \frac{G}{T} \right) \cdot \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right) \cdot \tilde{T}^{0.15} + \frac{E \left( \frac{G}{T} \right)^{0.20}}{F + \frac{G}{T}} \cdot \exp - \left( \frac{C}{T} \right)} \tag{5.24}
\]

where the derivatives to \(\tilde{\rho}\) and \(\tilde{T}\) are given by:

\[
\frac{\partial \tilde{D}_n}{\partial \tilde{\rho}} = - \frac{A \cdot H \left( F \tilde{T} + G \right)}{\tilde{\rho}^2 \left( J \left( F + \frac{G}{T} \right) \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right) \cdot \tilde{T}^{0.15} + \frac{E \left( \frac{G}{T} \right)^{0.20}}{F + \frac{G}{T}} \cdot \exp - \left( \frac{C}{T} \right) \right)} \tag{5.25}
\]

and

\[
\frac{\partial \tilde{D}_n}{\partial \tilde{T}} = \frac{A \cdot H}{\tilde{\rho}} \cdot \frac{F}{J \cdot \left( F + \frac{G}{T} \right) \cdot \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right) \cdot \tilde{T}^{0.15} + \frac{E \left( \frac{G}{T} \right)^{0.20}}{F + \frac{G}{T}} \cdot \exp - \left( \frac{C}{T} \right)} - \frac{A \cdot H \cdot \left( F \tilde{T} + G \right)}{\tilde{\rho}^2 \left( J \left( F + \frac{G}{T} \right) \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right) \cdot \tilde{T}^{0.15} + \frac{E \left( \frac{G}{T} \right)^{0.20}}{F + \frac{G}{T}} \cdot \exp - \left( \frac{C}{T} \right) \right)} \tag{5.26}
\]

\[
= - \frac{1.1J \cdot \left( F + \frac{G}{T} \right) \cdot C \cdot \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right)}{T^{1.95}} \cdot \left( \frac{0.15J \cdot \left( F + \frac{G}{T} \right) \cdot \exp - \left( \frac{C}{T^\frac{1}{1.15}} \right)}{T^{0.85}} + \frac{0.39E \cdot \exp - \left( \frac{C}{T} \right)}{T^2} \right) \tag{5.27}
\]

\[
+ \frac{E \cdot \left( \frac{G}{T} \right)^{0.20} \cdot G \cdot \exp - \left( \frac{C}{T} \right)}{T^2} \tag{5.28}
\]
5.5 Normalised Ionisation Energy

Per ionisation event an energy of $14.1 \text{eV}$ is needed. This amounts to $\xi = 14.1 \text{eV} = 2.26 \cdot 10^{-18} \text{J} = 6.75 \cdot 10^8 \frac{1}{\mu_0 \rho_0}$ (see Section 4.4 for an explanation of the conversions).

Applying proper normalisation gives

$$\tilde{\xi} = \mu_0 \rho_0 \xi = 2.839 \cdot 10^{-24} n_0$$

(5.31)
5.6 Reflective boundary condition

The reflective boundary condition

\[
(\rho v_{\parallel} - D_{\perp} \nabla \rho - (D_{\parallel} - D_{\perp}) \nabla _{\parallel} \rho) \cdot \mathbf{n} = D_n(\rho, \hat{T}) \nabla \rho_n \cdot \mathbf{n}
\]

(5.32)

is implemented separately at the divertor targets and the walls aligned with the flux surfaces.

5.6.1 Reflective boundary condition at divertor targets

At the divertor targets it is, in first instance, assumed that the convective flux dominates the diffusive flux so that the diffusive flux is ignored:

\[
(\rho v_{\parallel}) \cdot \mathbf{n} = D_n(\rho, \hat{T}) \nabla \rho_n \cdot \mathbf{n}
\]

(5.33)

At the divertor targets the normal vector (non normalized) can be defined as:

\[
\mathbf{n} = \nabla t = a^2
\]

(5.34)

For simplicity the normal vector is not normalized, since the inner product with the normal vector is taken at both sides of the equations. Writing

\[
\nabla \rho_n = \frac{\partial \rho_n}{\partial s} \nabla s + \frac{\partial \rho_n}{\partial t} \nabla t
\]

(5.35)

gives

\[
D_n(\rho, \hat{T}) \nabla \rho_n \cdot \mathbf{n} = D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial s} \nabla s \cdot \nabla t + D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial t} |\nabla t|^2
\]

(5.36)

In the code the vectorial parallel velocity is defined as a scalar $v_{\parallel}$ times the magnetic field $\mathbf{B}$ (see section about reduced MHD)

\[
v_{\parallel} = v_{\parallel} \mathbf{B}
\]

(5.37)

and $\mathbf{B}$ as

\[
\mathbf{B} = F_{\theta} \nabla \phi + \nabla \psi \times \nabla \phi
\]

(5.38)

Rewriting

\[
\nabla \psi = \frac{\partial \psi}{\partial s} \nabla s + \frac{\partial \psi}{\partial t} \nabla t + \frac{\partial \psi}{\partial \phi} \nabla \phi
\]

(5.39)

gives for

\[
\nabla \psi \times \nabla \phi = \frac{\partial \psi}{\partial s} \nabla s \times \nabla \phi + \frac{\partial \psi}{\partial t} \nabla t \times \nabla \phi = \frac{\partial \psi}{\partial s} \mathbf{a}_1 \cdot \mathbf{a}^3 + \frac{\partial \psi}{\partial t} \mathbf{a}_2 \cdot \mathbf{a}^3 = \frac{1}{J_3} \frac{\partial \psi}{\partial t} \mathbf{a}_1 - \frac{1}{J_3} \frac{\partial \psi}{\partial s} \mathbf{a}_2
\]

(5.40)

so that for $\mathbf{B} \cdot \mathbf{n}$ is found:

\[
\mathbf{B} \cdot \mathbf{n} = \frac{1}{J_3} \frac{\partial \psi}{\partial t} \mathbf{a}_1 \cdot \mathbf{a}^2 - \frac{1}{J_3} \frac{\partial \psi}{\partial s} \mathbf{a}_2 \cdot \mathbf{a}^2 = -\frac{1}{J_3} \frac{\partial \psi}{\partial s}
\]

(5.41)

which gives for $\rho v_{\parallel} \mathbf{B} \cdot \mathbf{n}$

\[
\rho v_{\parallel} \mathbf{B} \cdot \mathbf{n} = -\frac{\rho v_{\parallel}}{J_3} \frac{\partial \psi}{\partial s}
\]

(5.42)
Finally the boundary condition can be written as:

\[
\frac{\rho v_{\parallel}}{J_3} \frac{\partial \psi}{\partial s} = -D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial s} \nabla s \cdot \nabla t - D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial t} |\nabla t|^2
\]

(5.43)

Linearizing all variables (neglecting higher order derivatives)

\[
\frac{1}{J_3}(\rho_0 + \delta \rho)(v_{\parallel 0} + \delta v_{\parallel})(\left( \frac{\partial \psi}{\partial s} \right)_0 + \delta \frac{\partial \psi}{\partial s}) =

-D_n(\rho_0 + \delta \rho, \hat{T}_0 + \delta \hat{T}_0) \left( \frac{\partial \rho_n}{\partial s} \right)_0 \frac{\partial \rho_n}{\partial s} \nabla s \cdot \nabla t

-D_n(\rho_0 + \delta \rho, \hat{T}_0 + \delta \hat{T}_0) \left( \frac{\partial \rho_n}{\partial t} \right)_0 \frac{\partial \rho_n}{\partial t} |\nabla t|^2 =

-D_n(\rho_0 + \delta \rho, \hat{T}_0 + \delta \hat{T}_0) \left( \frac{\partial \rho_n}{\partial s} \right)_0 \frac{\partial \rho_n}{\partial s} \nabla s \cdot \nabla t

-D_n(\rho_0 + \delta \rho, \hat{T}_0 + \delta \hat{T}_0) \left( \frac{\partial \rho_n}{\partial t} \right)_0 \frac{\partial \rho_n}{\partial t} |\nabla t|^2 =

\]

(5.44)

results in the solution for the right hand side of the element matrix:

\[
- \frac{1}{J_3} \rho_0 v_{\parallel 0} \left( \frac{\partial \psi}{\partial s} \right)_0 - D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial s} \nabla s \cdot \nabla t - D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial t} |\nabla t|^2
\]

(5.45)

and the terms in the A-matrix:

\[
\delta \rho: \frac{1}{J_3} v_{\parallel 0} \left( \frac{\partial \psi}{\partial s} \right)_0 + \left( \frac{\partial D_n}{\partial \rho} \right)_{\rho_0, \hat{T}_0} \left( \frac{\partial \rho_n}{\partial s} \right)_0 \nabla s \cdot \nabla t + \left( \frac{\partial D_n}{\partial \rho} \right)_{\rho_0, \hat{T}_0} \left( \frac{\partial \rho_n}{\partial t} \right)_0 |\nabla t|^2
\]

(5.46)

\[
\delta \hat{T}: \left( \frac{\partial D_n}{\partial \hat{T}} \right)_{\rho_0, \hat{T}_0} \left( \frac{\partial \rho_n}{\partial s} \right)_0 \nabla s \cdot \nabla t + \left( \frac{\partial D_n}{\partial \hat{T}} \right)_{\rho_0, \hat{T}_0} \left( \frac{\partial \rho_n}{\partial t} \right)_0 |\nabla t|^2
\]

(5.47)

\[
\delta \frac{\partial \rho_n}{\partial s}: D_n(\rho_0, \hat{T}_0) \nabla s \cdot \nabla t
\]

(5.48)

\[
\delta \frac{\partial \rho_n}{\partial t}: D_n(\rho_0, \hat{T}_0) |\nabla t|^2
\]

(5.49)

\[
\delta v_{\parallel}: \frac{1}{J_3} \rho_0 \left( \frac{\partial \psi}{\partial s} \right)_0
\]

(5.50)

\[
\delta \frac{\partial \psi}{\partial s}: \frac{1}{J_3} \rho_0 v_{\parallel 0}
\]

(5.51)
5.6.2 Reflective boundary condition at boundaries parallel to the flux surfaces

At the boundaries parallel to the flux surfaces cross field diffusion dominates the outflow of plasma particles which results in the following boundary condition that it is to be applied at boundaries of this type:

\[-D_\perp \nabla \rho \cdot n = D_n(\rho, \hat{T}) \nabla \rho_n \cdot n\]  \hspace{1cm} (5.52)

At the boundaries parallel to the flux surfaces the normal vector can be defined as:

\[n = \nabla s = a^1\]  \hspace{1cm} (5.53)

where again the normal vector is not normalized since at the application of the boundary condition the inner product with the normal vector is taken at both sides of the equation.

With

\[\nabla \rho_n = \frac{\partial \rho_n}{\partial s} \nabla s + \frac{\partial \rho_n}{\partial t} \nabla t\]  \hspace{1cm} (5.54)

and

\[\nabla \rho_n = \frac{\partial \rho_n}{\partial s} \nabla s + \frac{\partial \rho_n}{\partial t} \nabla t\]  \hspace{1cm} (5.55)

Equation 5.52 can be written as

\[D_\perp \left( \frac{\partial \rho}{\partial s} \right)_0 |\nabla s|^2 + D_\perp \frac{\partial \rho}{\partial t} \nabla s \cdot \nabla t = -D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial s} |\nabla s|^2 - D_n(\rho, \hat{T}) \frac{\partial \rho_n}{\partial t} \nabla s \cdot \nabla t\]  \hspace{1cm} (5.56)

Linearizing the equation (disregarding higher order derivatives):

\[D_\perp \left( \frac{\partial \rho}{\partial s} \right)_0 \delta \rho + D_\perp \frac{\partial \rho}{\partial t} \delta \rho + \nabla \rho_n \cdot \nabla s = -D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial s} \delta \rho_n + D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial t} \delta \rho_n \nabla s \cdot \nabla t\]  \hspace{1cm} (5.57)

results in the solution for the right hand side of the element matrix:

\[-D_\perp \left( \frac{\partial \rho}{\partial s} \right)_0 |\nabla s|^2 - D_\perp \frac{\partial \rho}{\partial t} \nabla s \cdot \nabla t = -D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial s} |\nabla s|^2 - D_n(\rho_0, \hat{T}_0) \frac{\partial \rho_n}{\partial t} \nabla s \cdot \nabla t\]  \hspace{1cm} (5.58)

and the separate components of the A-matrix:

\[\delta \rho: \left( \frac{\partial D_n}{\partial \rho} \right)_{\rho_0, \hat{T}_0} \frac{\partial \rho_n}{\partial s} |\nabla s|^2 + \left( \frac{\partial D_n}{\partial \rho} \right)_{\rho_0, \hat{T}_0} \frac{\partial \rho_n}{\partial t} \nabla s \cdot \nabla t\]  \hspace{1cm} (5.59)
\[ \delta \hat{T}: \left( \frac{\partial D_n}{\partial \hat{T}} \right)_{\rho_0, \hat{T}_0} \frac{\partial \rho_n}{\partial s} |\nabla s|^2 + \left( \frac{\partial D_n}{\partial \hat{T}} \right)_{\rho_0, \hat{T}_0} \left( \frac{\partial \rho_n}{\partial t} \right)_{0} \nabla s \cdot \nabla t \] \hspace{1cm} (5.60)

\[ \delta \frac{\partial \rho}{\partial s}: D_{\perp} |\nabla s|^2 \] \hspace{1cm} (5.61)

\[ \delta \frac{\partial \rho}{\partial t}: D_{\perp} \nabla s \cdot \nabla t \] \hspace{1cm} (5.62)

\[ \delta \frac{\partial \rho_n}{\partial s}: D_{n}(\rho_0, \hat{T}_0) |\nabla s|^2 \] \hspace{1cm} (5.63)

\[ \delta \frac{\partial \rho_n}{\partial t}: D_{n}(\rho_0, \hat{T}_0) \nabla s \cdot \nabla t \] \hspace{1cm} (5.64)

### 5.6.3 Derivatives of boundary conditions

As outlined in Section 4.5.1 the degrees of freedom at every grid point are determined by the value of the variable, its derivatives in the s-direction and t-direction and its cross-derivative. At the divertor targets the finite elements are aligned with s at the geometrical boundary, so proper application of the reflective boundary condition here will also involve application of the derivative to s of the reflective boundary condition. Since calculating this derivative results in higher order terms this boundary condition cannot be applied this way. This is also the case for the derivative of the boundary condition at the boundary parallel to the magnetic flux surfaces. At first this seemed not to be a problem, but by increasing the amount of data points that were used in visualisation of the data it became clear that little spikes were present in the ingoing neutral flux (Section 6.2), which is a possible explanation for the particles lost in the plasma (Section 6.1). A workaround for proper application of the boundary conditions will have to be found.

### 5.6.4 Reflective boundary condition at corners points

At the corner points the boundary condition applied at both types of boundaries (at the divertor targets, Section 5.6.1, and at the boundaries parallel to the magnetic flux surfaces, Section 5.6.2) are added. In the simulations there have been a lot of problems with stability of the solution at the corner points. This has eventually been solved by one of two different approaches:

- Letting loose the plasma density at the boundaries parallel to the magnetic flux surfaces. This results in a slight increase of the plasma density in obtaining steady state. In former simulations this value always remained fixed.

- Applying an additional boundary condition for the derivative in the t-direction (the direction not parallel to the divertor plates) solves the problem with explosion of the solution at the corner points. The following boundary condition is applied:

\[ D_n \nabla \rho_n \cdot n_p = \frac{D \nabla \rho \cdot n_p}{(D \nabla \rho + \rho \nabla v) \cdot n_d} D_n \nabla \rho_n \cdot v \] \hspace{1cm} (5.65)

This additional equation ensures that the ratio of the ingoing flux at the divertor (type 1) to the ingoing flux in the direction of the boundary parallel to the magnetic flux surface (type 2) is equal to the ratio of the outgoing flux at the divertor to the outgoing flux in the direction of the boundary parallel to the magnetic flux surface. The reason for the need of the application of this boundary condition when the plasma density is kept fixed at the boundary parallel to the magnetic flux surface has not yet been found.
5.7 Weak form of the temperature equation

As outlined before (Equation 3.22) the evolution of the temperature is governed by the following equation:

$$\frac{\partial \hat{T}}{\partial t} = -\rho \mathbf{v} \cdot \nabla \hat{T} - (\gamma - 1)\rho \hat{T} \nabla \cdot \mathbf{v} - \hat{T} S_{\rho,\text{extra}} + S_{T,\text{extra}} - \hat{T} \rho \rho n_i(T) - \xi \rho \rho n_i(T) - \hat{T} \nabla \cdot \left( D_{\perp} \nabla \rho + (D_{\parallel} - D_{\perp}) \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \mathbf{B} \right) + \nabla \cdot \left( \kappa_{\perp} \nabla \hat{T} + (\kappa_{\parallel} - \kappa_{\perp}) \frac{\mathbf{B} \cdot \nabla \hat{T}}{B^2} \mathbf{B} \right)$$

Multiplying by a test function $T^*$ and integrating over the volume gives the weak form of this equation:

$$\int dV \left\{ T^* \rho \frac{\partial \hat{T}}{\partial t} \right\} =$$

$$\int dV \left\{ -\rho T^* \mathbf{v} \cdot \nabla \hat{T} - (\gamma - 1)\rho T^* \hat{T} \nabla \cdot \mathbf{v} - T^* \hat{T} S_{\rho,\text{extra}} + T^* S_{T,\text{extra}} \right\} +$$

$$\int dV \left\{ -T^* \hat{T} \rho n_i(T) - T^* \xi \rho n_i(T) \right\} +$$

$$\int dV \left\{ -T^* \hat{T} \nabla \cdot \left( D_{\perp} \nabla \rho + (D_{\parallel} - D_{\perp}) \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \mathbf{B} \right) \right\} +$$

$$\int dV \left\{ T^* \nabla \cdot \left( \kappa_{\perp} \nabla \hat{T} + (\kappa_{\parallel} - \kappa_{\perp}) \frac{\mathbf{B} \cdot \nabla \hat{T}}{B^2} \mathbf{B} \right) \right\}$$

(5.66)

In order to reduce continuity requirements the last two terms are rewritten by applying the product rule for divergence and the divergence theorem:

$$\int dV \left\{ T^* \rho \frac{\partial \hat{T}}{\partial t} \right\} =$$

$$\int dV \left\{ -\rho T^* \mathbf{v} \cdot \nabla \hat{T} - (\gamma - 1)\rho T^* \hat{T} \nabla \cdot \mathbf{v} - T^* \hat{T} S_{\rho,\text{extra}} + T^* S_{T,\text{extra}} \right\}$$

$$- \int dV \left\{ T^* \hat{T} \rho n_i(T) + T^* \xi \rho n_i(T) \right\}$$

$$+ \int dV \left\{ D_{\perp} T^* \nabla \rho \cdot \nabla \hat{T} + D_{\perp} \hat{T} \nabla \rho \cdot \nabla T^* \right\}$$

$$+ \int dV \left\{ (D_{\parallel} - D_{\perp}) T^* \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \left( \mathbf{B} \cdot \nabla \hat{T} \right) + (D_{\parallel} - D_{\perp}) T^* \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \left( \mathbf{B} \cdot \nabla T^* \right) \right\}$$

$$- \int dV \left\{ \kappa_{\perp} \nabla \hat{T} \cdot \nabla T^* + (\kappa_{\parallel} - \kappa_{\perp}) \frac{\mathbf{B} \cdot \nabla \hat{T}}{B^2} \left( \mathbf{B} \cdot \nabla T^* \right) \right\}$$

45
\[
- \int dS \left\{ T^* \hat{T} D_\perp \nabla \rho \cdot n + T^* \hat{T} (D_\parallel - D_\perp) \frac{(B \cdot \nabla \rho) (B \cdot n)}{B^2} \right\} \\
+ \int dS \left\{ T^* \kappa_\perp \nabla \hat{T} \cdot \n + T^* (\kappa_\parallel - \kappa_\perp) \frac{(B \cdot \nabla \hat{T}) (B \cdot n)}{B^2} \right\} \\
(5.67)
\]

In first instance the boundary term is omitted and boundary conditions are applied manually:

\[
\int dV \left\{ T^* \frac{\partial \hat{T}}{\partial t} \right\} = \\
\int dV \left\{ -\rho T^* \mathbf{v} \cdot \nabla \hat{T} - (\gamma - 1) \rho T^* \mathbf{v} \cdot \nabla \hat{T} S_{\rho,\text{extra}} + T^* S_{T,\text{extra}} \right\} \\
- \int dV \left\{ T^* \hat{T} \rho \rho S_\perp (\hat{T}) + T^* \xi \rho \rho S_\parallel (\hat{T}) \right\} \\
+ \int dV \left\{ D_\parallel T^* \nabla \rho \cdot \nabla \hat{T} + D_\parallel \nabla \rho \cdot \nabla T^* \right\} \\
+ \int dV \left\{ (D_\parallel - D_\perp) \hat{T} \frac{(B \cdot \nabla \rho) (B \cdot \nabla T^*)}{B^2} + (D_\parallel - D_\perp) T^* \frac{(B \cdot \nabla \rho) (B \cdot \nabla \hat{T})}{B^2} \right\} \\
- \int dV \left\{ \kappa_\perp \nabla \hat{T} \cdot \nabla T^* + (\kappa_\parallel - \kappa_\perp) \frac{(B \cdot \nabla \hat{T}) (B \cdot \nabla T^*)}{B^2} \right\} \\
(5.68)
\]

Applying the simplifications of reduced MHD and working out all the terms gives:

\[
-\rho T^* \mathbf{v} \cdot \nabla \hat{T} = T^* \rho R [\hat{T}, \mathbf{u}] - T^* \rho v_\parallel \frac{1}{R} [\hat{T}, \psi] - \rho v_\parallel T^* \frac{F_0 \partial \hat{T}}{R^2} \frac{\partial \phi}{\partial t} \]

\[
-(\gamma - 1) \rho TT^* \mathbf{v} \cdot \mathbf{v} = - (\gamma - 1) \left( \frac{F_0}{R^2} \rho \hat{T} \frac{\partial v_\parallel}{\partial \phi} + \frac{1}{R} \rho \hat{T} S_{\parallel, \text{extra}} + 2 \rho \hat{T} \frac{\partial \phi}{\partial t} \right) \]

\[
B \cdot \nabla \rho = \frac{F_0}{R^2} \frac{\partial \rho}{\partial \phi} + \frac{1}{R} [\rho, \psi] \\
(5.71)
\]

\[
B \cdot \nabla \hat{T} = \frac{F_0}{R^2} \frac{\partial \hat{T}}{\partial \phi} + \frac{1}{R} [\hat{T}, \psi] \\
(5.72)
\]

\[
B \cdot \nabla T^* = \frac{F_0}{R^2} \frac{\partial T^*}{\partial \phi} + \frac{1}{R} [T^*, \psi] \\
(5.73)
\]

\[
B^2 = \frac{1}{R^2} \left( F_0 + \left( \frac{\partial \psi}{\partial x} \right)^2 + \left( \frac{\partial \psi}{\partial y} \right)^2 \right) \\
(5.74)
\]
5.7.1 Cranck-Nicholson Formulation

Restating the Cranck-Nicholson formulation specifically for the temperature equation

\[ \rho_0 T^* \delta \hat{T} - \frac{1}{2} \sum_{i=1}^{8} \left( \frac{\partial A}{\partial y_i} \right) v \delta y_i = \delta t A_0 \]  

(5.75)

gives for the relevant components of A (only the components that result from the density diffusion term, the density source term and the temperature source term as a result of ionization are listed, hence the expression \( A^+ \) denoting that the certain terms are not listed)

\[ A^+ = \]

\[-T^* \xi(\rho, \hat{T}) S_i(\hat{T}) \rho \rho_n \]

\[-T^* \hat{T} S_i(\hat{T}) \rho \rho_n \]

\[+ D_\perp \hat{T} \nabla \rho \cdot \nabla T^* \]

\[+ D_\perp T^* \nabla \rho \cdot \nabla \hat{T} \]

\[+(D_\parallel - D_\perp) \hat{T} \frac{(B \cdot \nabla T^*)(B \cdot \nabla \rho)}{B^2} \]

\[+(D_\parallel - D_\perp) T^* \frac{(B \cdot \nabla \hat{T})(B \cdot \nabla \rho)}{B^2} \]  

(5.76)

so that for \( A_0 \) is found

\[ A_{0^+} = \]

\[-T^* \xi(\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_0 \rho_{0n} \]

\[-T^* \hat{T}_0 S_i(\hat{T}_0) \rho_0 \rho_{0n} \]

\[+ D_\perp \hat{T}_0 \nabla \rho_0 \cdot \nabla T^* \]

\[+ D_\perp T^* \nabla \rho_0 \cdot \nabla \hat{T}_0 \]

\[+(D_\parallel - D_\perp) \hat{T}_0 \frac{(B_0 \cdot \nabla T^*)(B_0 \cdot \nabla \rho_0)}{B_0^2} \]

\[+(D_\parallel - D_\perp) T^* \frac{(B_0 \cdot \nabla \hat{T}_0)(B_0 \cdot \nabla \rho_0)}{B_0^2} \]  

(5.77)

The derivative of A to \( \psi \) gives

\[ \left( \frac{\partial A}{\partial \psi} \right)_0^+ = \]

\[-(D_\parallel - D_\perp) T^* \frac{(B_0 \cdot \nabla \hat{T}_0)(B_0 \cdot \nabla \rho_0)}{B_0^2} \left( \frac{\partial B^2}{\partial \psi} \right) \psi_0 \]

\[+(D_\parallel - D_\perp) T^* \frac{(\frac{\partial B}{\partial \psi}) \psi_0 \cdot \nabla \hat{T}_0 (B_0 \cdot \nabla \rho_0)}{B_0^2} \]

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\[ + (D_{\parallel} - D_{\perp}) T^* \frac{(B_0 \cdot \nabla \hat{T}_0)}{B_0^2} \left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \cdot \nabla \rho_0 \]

\[ - (D_{\parallel} - D_{\perp}) \hat{T}_0 \frac{(B_0 \cdot \nabla T^*)(B_0 \cdot \nabla \rho_0)}{B_0^2} \left( \frac{\partial B^2}{\partial \psi} \right)_{\psi_0} \]

\[ + (D_{\parallel} - D_{\perp}) \hat{T}_0 \left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \cdot \nabla T^* \left( B_0 \cdot \nabla \rho_0 \right) \]

\[ + (D_{\parallel} - D_{\perp}) \hat{T}_0 \left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \cdot \nabla \rho_0 \]

\[ + (D_{\parallel} - D_{\perp}) \hat{T}_0 \frac{(B_0 \cdot \nabla T^*)(B_0 \cdot \nabla \rho_0)}{B_0^2} \]

The derivative of \(A\) to \(\rho\) gives

\[ \left( \frac{\partial A}{\partial \rho} \right)_{\rho_0} = \]

\[ - T^* \xi(\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_{a0} - T^* \left( \frac{\partial \xi}{\partial \hat{T}} \right)_{(\rho_0, \hat{T}_0)} S_i(\hat{T}_0) \rho_{a0} \]

\[ - T^* \hat{T}_0 S_i(\hat{T}_0) \rho_{a0} \]

\[ + D_{\perp} \hat{T}_0 \nabla T^* \cdot \nabla \]

\[ + D_{\perp} T^* \nabla \hat{T}_0 \cdot \nabla \]

\[ + (D_{\parallel} - D_{\perp}) \hat{T}_0 \frac{(B_0 \cdot \nabla T^*)(B_0 \cdot \nabla)}{B_0^2} \]

\[ + (D_{\parallel} - D_{\perp}) T^* \frac{(B_0 \cdot \nabla \hat{T}_0)(B_0 \cdot \nabla)}{B_0^2} \]

The derivative to \(\hat{T}\) gives

\[ \left( \frac{\partial A}{\partial \hat{T}} \right)_{\hat{T}_0} = \]

\[ - T^* \left( \frac{\partial \xi}{\partial \hat{T}} \right)_{(\rho_0, \hat{T}_0)} S_i(\hat{T}_0) \rho_{a0} - T^* \xi(\rho_0, \hat{T}_0) \left( \frac{\partial S_i(\hat{T})}{\partial \hat{T}} \right)_{\hat{T}_0} \rho_{a0} \]

\[ - T^* S_i(\hat{T}_0) \rho_{a0} - T^* \hat{T}_0 \left( \frac{\partial S_i(\hat{T})}{\partial \hat{T}} \right)_{\hat{T}_0} \rho_{a0} \]

\[ + D_{\perp} \nabla \rho_0 \cdot \nabla T^* \]

\[ + D_{\perp} T^* \nabla \rho_0 \cdot \nabla \]

\[ + (D_{\parallel} - D_{\perp}) \frac{(B_0 \cdot \nabla T^*)(B_0 \cdot \nabla \rho_0)}{B_0^2} \]

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\[(D_\parallel - D_\perp)T^* \frac{(\mathbf{B}_0 \cdot \nabla \rho_0)(\mathbf{B}_0 \cdot \nabla)}{B_0^2}\]  

and finally the derivative to \(\rho_n\) gives
\[\left(\frac{\partial A}{\partial \rho}\right)_0 =
-T^* \xi(\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_0
- T^* \hat{T}_0 S_i(\hat{T}_0) \rho_0
\]

so that as additional terms for the RHS of equation 6 are found:

\[\text{RHS}_6 =
-T^* \xi(\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_0 \rho_n 0
+ D_\perp \hat{T}_0 \nabla \rho_0 \cdot \nabla T^*
+ D_\perp T^* \nabla \rho_0 \cdot \nabla \hat{T}_0
+ (D_\parallel - D_\perp) \hat{T}_0 \frac{(\mathbf{B}_0 \cdot \nabla T^*)(\mathbf{B}_0 \cdot \nabla \rho_0)}{B_0^2}
+ (D_\parallel - D_\perp) T^* \frac{(\mathbf{B}_0 \cdot \nabla \hat{T}_0)(\mathbf{B}_0 \cdot \nabla \rho_0)}{B_0^2}\]

and separating the left hand side for each variable (again only additional terms, the components that result from the density diffusion term, the density source term and the temperature source term as a result of ionization, are listed), first all terms involving \(\delta \psi\):

\[\text{amat}_6 =
\frac{1}{2}(D_\parallel - D_\perp)T^* \frac{(\mathbf{B}_0 \cdot \nabla \hat{T}_0)(\mathbf{B}_0 \cdot \nabla \rho_0)}{B_0^2} \left(\frac{\partial B^2}{\partial \psi}\right)_0 \delta \psi
- \frac{1}{2}(D_\parallel - D_\perp)T^* \frac{\left(\frac{\partial \mathbf{B}}{\partial \psi}\right)_0 \delta \psi \cdot \nabla \hat{T}_0}{B_0^2} (\mathbf{B}_0 \cdot \nabla \rho_0)
+ \frac{1}{2}(D_\parallel - D_\perp) \hat{T}_0 \frac{(\mathbf{B}_0 \cdot \nabla T^*)(\mathbf{B}_0 \cdot \nabla \rho_0)}{B_0^2} \left(\frac{\partial B^2}{\partial \psi}\right)_0 \delta \psi
- \frac{1}{2}(D_\parallel - D_\perp) \hat{T}_0 \left(\frac{\partial \mathbf{B}}{\partial \psi}\right)_0 \delta \psi \cdot \nabla T^* (\mathbf{B}_0 \cdot \nabla \rho_0)\]

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\[
- \frac{1}{2}(D_{\parallel} - D_{\perp})\hat{T}_0 \frac{(\mathbf{B}_0 \cdot \nabla T^*) \left( \frac{\partial \mathbf{B}}{\partial \psi} \delta \psi \cdot \nabla \rho_0 \right)}{B^2_0} \] (5.82)

, terms involving \( \delta \rho \)

\[
\frac{\text{amat}_{65}}{\delta t \text{RJ}_2} = +
\frac{1}{2} T^* \xi (\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_{00} \delta \rho + \frac{1}{2} T^* \left( \frac{\partial \xi}{\partial \rho} \right)_{(\rho_0, \hat{T}_0)} S_i(\hat{T}_0) \rho_{00} \rho_{00} \delta \rho
\]

\[
+ \frac{1}{2} T^* \hat{T}_0 S_i(\hat{T}_0) \rho_{00} \delta \rho
\]

\[
- \frac{1}{2} D_{\perp} \nabla T^* \cdot \nabla \rho
\]

\[
- \frac{1}{2} D_{\perp} T^* \nabla \hat{T}_0 \cdot \nabla \rho
\]

\[
- \frac{1}{2} (D_{\parallel} - D_{\perp})\hat{T}_0 \frac{(\mathbf{B}_0 \cdot \nabla T^*) (\mathbf{B}_0 \cdot \nabla \delta \rho)}{B^2_0}
\]

(5.83)

, terms involving \( \delta \hat{T} \)

\[
\frac{\text{amat}_{66}}{\delta t \text{RJ}_2} = +
\frac{1}{2} T^* \left( \frac{\partial \xi}{\partial T} \right)_{(\rho_0, \hat{T}_0)} S_i(\hat{T}_0) \rho_{00} \rho_{00} \delta \hat{T} + \frac{1}{2} T^* \xi (\rho_0, \hat{T}_0) \left( \frac{\partial S_i(\hat{T})}{\partial T} \right)_{\hat{T}_0} \rho_{00} \rho_{00} \delta \hat{T}
\]

\[
+ \frac{1}{2} T^* S_i(\hat{T}_0) \rho_{00} \rho_{00} \delta \hat{T} + \frac{1}{2} T^* \hat{T}_0 \left( \frac{\partial S_i(\hat{T})}{\partial T} \right)_{\hat{T}_0} \rho_{00} \rho_{00} \delta \hat{T}
\]

\[
- \frac{1}{2} D_{\perp} \nabla \rho \cdot \nabla T^* \delta \hat{T}
\]

\[
- \frac{1}{2} D_{\perp} T^* \nabla \rho \cdot \nabla \delta \hat{T}
\]

\[
- \frac{1}{2} (D_{\parallel} - D_{\perp})\frac{(\mathbf{B}_0 \cdot \nabla T^*) (\mathbf{B}_0 \cdot \nabla \rho)}{B^2_0} \delta \hat{T}
\]

\[
- \frac{1}{2} (D_{\parallel} - D_{\perp}) T^* \frac{(\mathbf{B}_0 \cdot \nabla \rho) (\mathbf{B}_0 \cdot \nabla \delta \hat{T})}{B^2_0}
\]

(5.84)

and finally terms involving \( \delta \rho_n \)

\[
\frac{\text{amat}_{68}}{\delta t \text{RJ}_2} = +
\frac{1}{2} T^* \xi (\rho_0, \hat{T}_0) S_i(\hat{T}_0) \rho_0 \delta \rho_n
\]

\

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\[ + \frac{1}{2} T^* \hat{T}_0 S_1(\hat{T}_0) \rho_0 \delta \rho_n \]

with

\[
\left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \delta \psi \cdot \nabla \hat{T}_0 = \frac{1}{R} [\hat{T}_0, \delta \psi] \quad (5.85)
\]

\[
\left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \delta \psi \cdot \nabla T^* = \frac{1}{R} [T^*, \delta \psi] \quad (5.86)
\]

\[
\left( \frac{\partial B}{\partial \psi} \right)_{\psi_0} \delta \psi \cdot \nabla \rho = \frac{1}{R} [\rho, \delta \psi] \quad (5.87)
\]

\[
B \cdot \nabla \delta \hat{T} = \frac{F_0}{R^2} \frac{\partial \delta \hat{T}}{\partial \phi} + \frac{1}{R} [\delta \hat{T}, \psi] \quad (5.88)
\]

\[
B \cdot \nabla \delta \rho = \frac{F_0}{R^2} \frac{\partial \delta \rho}{\partial \phi} + \frac{1}{R} [\delta \rho, \psi] \quad (5.89)
\]

\[
\frac{\partial B^2}{\partial \psi \cdot \delta \psi} = \frac{2}{R^2} \left( \frac{\partial \psi \partial \delta \psi}{\partial x \cdot \partial x} + \frac{\partial \psi \partial \delta \psi}{\partial y \cdot \partial y} \right) \quad (5.90)
\]
5.8 Weak form of the neutral density equation

As outlined in Equation 5.91 the neutral density is governed by the following equation:

$$\frac{\partial \rho_n}{\partial t} = + \nabla \cdot (D_n(\rho, \hat{T}) \nabla \rho_n) - \rho_n \rho \rho_n S_i(\hat{T}) + S_{\text{neutral,extra}}$$  \hspace{1cm} (5.91)

Multiplying by a test function $\rho_n^*$ and integrating over the volume $V$ gives the weak form of this equation:

$$\int dV \left\{ \rho_n^* \frac{\partial \rho_n}{\partial t} \right\} =$$

$$\int dV \left\{ \rho_n^* \nabla \cdot (D_n(\rho, \hat{T}) \nabla \rho_n) - \rho_n^* \rho \rho_n S_i(\hat{T}) + \rho_n^* S_{\text{neutral,extra}} \right\}$$  \hspace{1cm} (5.92)

Reducing continuity requirements by applying the product rule for divergence and the divergence theorem:

$$\int dV \left\{ \rho_n^* \frac{\partial \rho_n}{\partial t} \right\} =$$

$$\int dV \left\{ - D_n(\rho, \hat{T}) \nabla \rho_n \cdot \nabla \rho_n^* - \rho_n^* \rho \rho_n S_i(\hat{T}) + \rho_n^* S_{\text{neutral,extra}} \right\}$$

$$\int dS \left\{ \rho_n^* D_n(\rho, \hat{T}) \nabla \rho_n \cdot \hat{n} \right\}$$  \hspace{1cm} (5.93)

In first instance the boundary integral is omitted and the boundary conditions are applied manually, which results in the following final weak form of the neutral fluid equation:

$$\int dV \left\{ \rho_n^* \frac{\partial \rho_n}{\partial t} \right\} =$$

$$\int dV \left\{ - D_n(\rho, \hat{T}) \nabla \rho_n \cdot \nabla \rho_n^* - \rho_n^* \rho \rho_n S_i(\hat{T}) + \rho_n^* S_{\text{neutral,extra}} \right\}$$  \hspace{1cm} (5.94)

5.8.1 Cranck-Nicholson Formulation

Restating the Cranck-Nicholson formulation specifically for the neutral fluid equation

$$\rho_n^* \delta \rho_n - \frac{1}{2} \sum_{i=1}^{8} \left( \frac{\partial A}{\partial y_i} \right)_0 \delta y_i = \delta t A_0$$  \hspace{1cm} (5.95)

where $A$ is given by

$$A = - D_n(\rho, \hat{T}) \nabla \rho_n \cdot \nabla \rho_n^* - \rho_n^* \rho \rho_n S_i(\hat{T}) + \rho_n^* S_{\text{neutral,extra}}$$  \hspace{1cm} (5.96)

so that for $A_0$ is found:

$$A_0 = - D_n(\rho_0, \hat{T}_0) \nabla \rho_{n0} \cdot \nabla \rho_n^* - \rho_n^* \rho_0 \rho_{n0} S_i(\hat{T}_0) + \rho_n^* S_{\text{neutral,extra}}$$  \hspace{1cm} (5.97)

$$A_0 = - D_n(\rho_0, \hat{T}_0) \nabla \rho_{n0} \cdot \nabla \rho_n^* - \rho_n^* \rho_0 \rho_{n0} S_i(\hat{T}_0) + \rho_n^* S_{\text{neutral,extra}}$$  \hspace{1cm} (5.98)

For simplicity a constant extra neutral source term is assumed which gives rise to the following derivatives:

$$\left( \frac{\partial A}{\partial \psi} \right)_0 = \left( \frac{\partial A}{\partial u} \right)_0 = \left( \frac{\partial A}{\partial j} \right)_0 = \left( \frac{\partial A}{\partial w} \right)_0 = \left( \frac{\partial A}{\partial v} \right)_0 = 0$$  \hspace{1cm} (5.99)
\[
\frac{\partial A}{\partial \rho} = -\left( \frac{\partial D_n}{\partial \rho} \right)_{\rho_0, \hat{T}_0} \nabla \rho^*_n \cdot \nabla \rho_n - \rho^*_n \rho_n S_i(\hat{T}_0) \tag{5.100}
\]

\[
\frac{\partial A}{\partial \hat{T}} = -\left( \frac{\partial D_n}{\partial \hat{T}} \right)_{\rho_0, \hat{T}_0} \nabla \rho^*_n \cdot \nabla \rho_n - \rho^*_n \rho_n \left( \frac{\partial S_i}{\partial \hat{T}} \right)_{\hat{T}_0} \tag{5.101}
\]

\[
\frac{\partial A}{\partial \rho_n} = -D_n(\rho_0, \hat{T}_0) \nabla \rho^*_n \cdot \nabla - \rho^*_n \rho S_i(\hat{T}_0) \tag{5.102}
\]

For the right hand side (RHS) of the neutral fluid equation is found:

\[
\text{RHS}_{8} = -D_n(\rho_0, \hat{T}_0) \nabla \rho^*_n \cdot \nabla \rho_n - \rho^*_n \rho_0 \rho_{n0} S_i(\hat{T}_0) + \rho^*_n S_{\text{neutral, extra}} \tag{5.103}
\]

and for the A-matrix:

\[
\frac{\text{amat}_{85}}{\delta tRJ_2} = -\frac{1}{2} \frac{\partial D_n}{\partial \rho} (\nabla \rho^*_n \cdot \nabla \rho_n) \delta \rho - \frac{1}{2} \rho^*_n \rho_n S_i(\hat{T}) \delta \rho \tag{5.104}
\]

\[
\frac{\text{amat}_{86}}{\delta tRJ_2} = -\frac{1}{2} \frac{\partial D_n}{\partial \hat{T}} (\nabla \rho^*_n \cdot \nabla \rho_n) \delta \hat{T} - \frac{1}{2} \rho^*_n \rho_n \frac{\partial S_i}{\partial \hat{T}} \delta \hat{T} \tag{5.105}
\]

\[
\frac{\text{amat}_{88}}{\delta tRJ_2} = \rho^*_n \delta \rho_n - \frac{1}{2} D_n(\rho_0, \hat{T}_0) \nabla \rho^*_n \cdot \nabla \delta \rho_n - \frac{1}{2} \rho^*_n \rho S_i(\hat{T}) \delta \rho_n \tag{5.106}
\]

where

\[
\nabla \rho^*_n \cdot \nabla \rho_n = \frac{\partial \rho^*_n}{\partial x} \frac{\partial \rho_n}{\partial x} + \frac{\partial \rho^*_n}{\partial y} \frac{\partial \rho_n}{\partial y} + \frac{\partial \rho^*_n}{\partial \phi} \frac{\partial \rho_n}{\partial \phi} \tag{5.107}
\]

and

\[
\nabla \rho^*_n \cdot \nabla \delta \rho_n = \frac{\partial \rho^*_n}{\partial x} \frac{\partial \delta \rho_n}{\partial x} + \frac{\partial \rho^*_n}{\partial y} \frac{\partial \delta \rho_n}{\partial y} + \frac{\partial \rho^*_n}{\partial \phi} \frac{\partial \delta \rho_n}{\partial \phi} \tag{5.108}
\]
5.9 Weak form of the plasma fluid density equation

As outlined in Equation 3.17 the neutral density is governed by the following equation:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) + \nabla \cdot (D_{\perp} \nabla \rho + D_{\parallel} \nabla \rho) + \rho \rho_n S_i(\tilde{T}) + S_{\text{plasma,extra}}$$  \hspace{1cm} (5.109)

Besides the ionization term, this equation is already successfully implemented in JOREK. To be complete the full form of the weak form of this equation is deduced again. In determining the relevant terms for the right hand sides and the A-matrix the terms already implemented will be omitted.

Rewriting the diffusive flux in a component parallel to the magnetic field and a component of the full density gradient gives:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) + \nabla \cdot (D_{\perp} \nabla \rho) + (D_{\parallel} - D_{\perp}) \mathbf{B} \cdot \nabla \rho \frac{\mathbf{B}}{B^2} + \rho \rho_n S_i(\tilde{T}) + S_{\text{plasma,extra}}$$  \hspace{1cm} (5.110)

Multiplying by a test function $\rho^*$ and integrating over the volume $V$ gives the weak form of this equation:

$$\int dV \left\{ \rho^* \frac{\partial \rho}{\partial t} \right\} =$$

$$\int dV \left\{ -\rho^* \nabla \cdot (\rho \mathbf{u}) + \rho^* \nabla \cdot (D_{\perp} \nabla \rho) \right\} +$$

$$\int dV \left\{ \rho^* \rho \rho_n S_i(\tilde{T}) + \rho^* S_{\text{plasma,extra}} \right\}$$  \hspace{1cm} (5.111)

Reducing continuity requirements by applying the product rule for divergence and the divergence theorem:

$$\int dV \left\{ \rho^* \frac{\partial \rho}{\partial t} \right\} =$$

$$\int dV \left\{ -\rho^* \nabla \cdot (\rho \mathbf{u}) - D_{\perp} \nabla \rho \cdot \nabla \rho^* - (D_{\parallel} - D_{\perp}) \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \right\} +$$

$$\int dV \left\{ \rho^* \rho \rho_n S_i(\tilde{T}) + \rho^* S_{\text{plasma,extra}} \right\}$$

$$\int dS \left\{ \rho^* D_{\perp} \nabla \rho \cdot \mathbf{n} + \rho^* (D_{\parallel} - D_{\perp}) \frac{\mathbf{B} \cdot \nabla \rho (\mathbf{B} \cdot \mathbf{n})}{B^2} \right\}$$  \hspace{1cm} (5.112)

In first instance the boundary integral is omitted and the boundary conditions are applied manually, which results in the following final weak form of the plasma density equation:

$$\int dV \left\{ \rho^* \frac{\partial \rho}{\partial t} \right\} =$$

$$\int dV \left\{ -\rho^* \nabla \cdot (\rho \mathbf{u}) - D_{\perp} \nabla \rho \cdot \nabla \rho^* - (D_{\parallel} - D_{\perp}) \frac{\mathbf{B} \cdot \nabla \rho}{B^2} \right\} +$$

$$\int dV \left\{ \rho^* \rho \rho_n S_i(\tilde{T}) + \rho^* S_{\text{plasma,extra}} \right\}$$  \hspace{1cm} (5.113)
5.9.1 Cranck-Nicholson Formulation

Restating the Cranck-Nicholson formulation specifically for the plasma density equation

\[ \rho^* \delta \rho - \frac{1}{2} \sum_{i=1}^{8} \left( \frac{\partial A}{\partial y_i} \right)_0 \delta y_i = \delta t A_0 \]  \hspace{1cm} (5.114)

where the additional term due to ionized neutrals in \( A \) is given by

\[ A^+ = \rho^* \rho \rho_n S_i \hat{T} \]  \hspace{1cm} (5.115)

which results in

\[ A_{0+} = \rho^* \rho_0 \rho_{n0} S_i \hat{T}_0 \]  \hspace{1cm} (5.116)

This term gives rise to the following derivatives:

\[ \left( \frac{\partial A}{\partial \psi} \right)_0 + = \left( \frac{\partial A}{\partial u} \right)_0 + = \left( \frac{\partial A}{\partial j} \right)_0 + = \left( \frac{\partial A}{\partial v} \right)_0 + = 0 \]  \hspace{1cm} (5.117)

\[ \left( \frac{\partial A}{\partial \rho} \right)_0 + = \rho^* \rho_{n0} S_i \hat{T}_0 \]  \hspace{1cm} (5.118)

\[ \left( \frac{\partial A}{\partial \hat{T}} \right)_0 + = \rho^* \rho_0 \rho_{n0} \left( \frac{\partial S_i}{\partial \hat{T}} \right) \hat{T}_0 \]  \hspace{1cm} (5.119)

\[ \left( \frac{\partial A}{\partial \rho_n} \right)_0 + = \rho^* \rho_0 S_i \hat{T}_0 \]  \hspace{1cm} (5.120)

For the right hand side (RHS) of the ionization term in the plasma continuity equation is found:

\[ \frac{\text{RHS}_5}{\delta t R J_2} + = \rho^* \rho_0 \rho_{n0} S_i \hat{T}_0 \]  \hspace{1cm} (5.121)

and for the terms in the \( A \)-matrix:

\[ \frac{\text{amat}_{55}}{\delta t R J_2} + = \rho^* \rho_{n0} S_i \hat{T}_0 \delta \rho \]  \hspace{1cm} (5.122)

\[ \frac{\text{amat}_{56}}{\delta t R J_2} + = \rho^* \rho_0 \rho_{n0} \left( \frac{\partial S_i}{\partial \hat{T}} \right) \hat{T}_0 \delta \hat{T} \]  \hspace{1cm} (5.123)

\[ \frac{\text{amat}_{58}}{\delta t R J_2} + = \rho^* \rho_0 S_i \hat{T}_0 \delta \rho_n \]  \hspace{1cm} (5.124)
Verification of Code

Several methods can be used to verify the code. Firstly the amount of particles has to be conserved, since all plasma particles are reflected as neutrals and since a positively inward gradient of neutrals is present at all points, no neutrals will leave the plasma. Secondly since a reflective boundary condition is applied the inward neutral flux has to be equal to the outward plasma flux. Thirdly the neutral penetration depth can be compared to its theoretical prediction. Fourthly the neutral profile can be compared to generated profiles in specialized 2D-divertor codes in similar conditions. A fifth way to check correct implementation is a slight drop of temperature and pressure near the divertor target, because of consumed energy going along with the ionisation of neutrals, that should match similar calculations in other codes. Sixth, there should be a rise in density towards the divertor targets, because of ionisation of neutrals, which should also match similar calculations in other codes. As a seventh way to check correct implementation; convergence of the amount of particles that is lost over the course of a definite amount of timesteps must result from an increasing resolution in either grid size or timestep.

6.1 Conservation of Particles and Convergency Tests

Two types of simulations have been performed to check for particle conservation. One in circular toroidal geometry and one in a toroidal geometry with an X-point and divertor targets. Both types of simulations start from a certain set of initial conditions with no neutral particles. In circular toroidal geometry a run of 500 Alfven time steps has been performed in a resolution of 41 elements in the radial direction and 64 elements in the poloidal direction. One situation with the ionisation particle source term turned on and one situation with the particle flux turned off are run. In both cases the total amount of lost particles is less than 1% of the outward particle flux (assuming the outward particle flux in the case of the ionisation source activated is of the same order as the outward particle flux in the case of the ionisation source turned off), see Figure 6.1. In the x-point plasma the loss is substantially more (about 10%-20% of the outward flux in the applicable resolution). This is an unexpected result, since the plasma particles flowing out of the plasma should entirely be recycled as neutrals. It was unclear for a long time, what resulted in the loss of particles, but the explanation is probably to be found in the improper application of the reflective boundary condition, due to the fact that the derivative of the boundary condition is not being applied (see Section 5.6.3). This will have to be verified in the future and a workaround for proper application of the derivative of the boundary condition will have to be sought for.
6.1.1 Convergency Tests

Increasing grid resolution and timestep will have to improve the loss fraction of particles. Two situations are considered, one in circular geometry and one in x-point geometry. In Figure 6.3 there is shown that the loss fraction decreases linearly with decreasing time step (though absolute dependency on time step is very small due to the implicit Cranck-Nicholson approach). In Figure 6.4 an increase in particle conservation is observed when the resolution in poloidal direction is increased. Due to the fact that the derivative of the reflective boundary condition is not applied, the resolution in the C-direction in X-point geometry has a significant influence on the particle conservation ratio as pictured in Figure 6.5. Also an increase in resolution in the D-direction and E-direction significantly improves particle conservation (Figure 6.6 and Figure 6.7, see Section 4.1 for an explanation of the C,D and E directions).

6.2 Comparison of outward and inward flux

Data generated in Jorek can be visualised by converting the generated data to a vtk-file that is readable in the data visualisation packet Paraview. The values of the variables on the grid points are usually visualised, but when higher visualisation resolution is required also values between grid points can be generated (based on the derivatives between grid points). In Figure 6.8 the outward plasma flux is shown and is equal for visualisation of the outward flux at the grid points only and for visualisation at grid points including 3 points in between grid points.

In Figure 6.9 the inward flux visualised at grid points only is shown. Mapping over the inward and outward fluxes shows them to be equal and proves proper application of the reflective boundary condition at the grid points at the divertor targets.
In Figure 6.2 the inward flux visualised at the grid points and at 3 points in between the grid points is pictured. The spikes result from improper application of the derivative of the boundary condition in the direction parallel to the divertor targets. A workaround will have to be sought in order to correct this which will probably also result in particle conservation. The data shown in Figure 6.8 and Figure 6.10 visualises the same situation. The situation shown in Figure 6.9 shows a different situation, so only a rough comparison can be made. Data visualising the outward flux,
Figure 6.4: Particle loss fraction as a function of increasing poloidal resolution. Increasing the poloidal resolution beyond 60-80 has no more significant effect.

Figure 6.5: Particle loss fraction as a function of increasing resolution in C-direction (X-point geometry). The particle loss fraction is extremely sensitive on the resolution alongside the divertor targets.

the inward flux at the grid points only and the inward flux at the grid points including 3 points in between the grid points in the same run is currently unavailable.

6.3 Neutral Penetration Depth

The neutral penetration depth is given by [US04]:

\[
\lambda_n,\text{penetration} = \frac{\nu_{th}}{n_e \sqrt{<\sigma v>_{\text{c.e.}} <\sigma v>_{\text{ionisation}}}}
\]  

(6.1)
A case has been run with a particle density of $1.5 \cdot 10^{20}$ and a temperature $T = T_i = T_e$ at the divertor targets. This amounts to a neutral penetration depth of $\lambda_{n,\text{penetration}} = 1.8\text{cm}$. As shown in Figure 6.11 the neutral penetration depth is approximately 1.8cm (rough estimation) which agrees with the theoretical prediction.
6.4 Specialised 2D Divertor Code Comparisons

A comparison case of a simulation in a JET 50401 run with EDGED2D-Eirene has been used. EDGE2D solves the fluid equations for the conservation of particles, momentum and energy for
hydrogenic and impurity ions, while neutrals are followed with the two-dimensional Monte Carlo module EIRENE. External boundary conditions from experiment are used. The plasma cross-field diffusion coefficient in the SOL was set at 0.1m²/s and heat conductivities \( \chi_{Le} = \chi_{Li} = 1.0m²/s \). The parallel conductivities scale Spitzer Harm like. The grid covers the SOL, the private flux zone and some of the closed flux surfaces (a few centimetres at outer-midplane). The run is performed in a geometry with vertical divertor targets (contrary to the geometry of the divertor targets in JOREK). In both cases the temperature at the divertor targets is approximately 70eV, see Figure 6.12 a.) (in the Jorek case this is the plasma temperature which is taken to be equal to the electron temperature and the ion temperature in the calculation of the neutral diffusion coefficient. In the JET 50401 run this represents the electron temperature). Values are not exact, but approximated and exact values will have to be validated. Another comparison case in proper geometry with equal density, temperature and inward neutral flux will finally have to validate the correct implementation of the neutral fluid model.

The density at the divertor targets is slightly higher in the JOREK Run, \( n_{\text{Divertor Target Jorek}} = 1.5 \cdot 10^{20} \) than in the JET run, \( n_{\text{Divertor Target EDGE2DEirene}} = 5 \cdot 10^{19} \) which will cause the neutrals to penetrate less deeply into the plasma in the JOREK run. This is indeed observed, as the shape of the curve of the fall-off of the neutral density is similar in both cases and the e-folding length in the EDGE2DEirene run is longer (approximately 5.4cm). Values shown are roughly estimated. More exact values will have to be extracted when a better comparison case is being performed.

### 6.5 Temperature Drop towards Divertor Targets

Due to the energy consumed at ionisation events a small temperature and pressure decrease is expected at the divertor targets. As shown in Figure 6.13 the contrary is observed. It is highly likely that this is happening because of the fact that terms are added to the wrong position in the matrix. A future run will have to confirm this assumption.

### 6.6 Density Rise towards Divertor Targets

Due to ionisation of reflected neutrals there is a slight rise in density expected towards the divertor targets, which is indeed observed as pictured in Figure 6.14 which shows the steady-state density solution at the outer divertor target.
Figure 6.12: Comparison Case (left: JOREK Run, right: EDGED2D-Eirene JET Run). Profiles are similar and the e-folding length in the EDGE2D run is approximately 3 times higher than in the JOREK run which is expected due to the fact that the plasma density is 3 times higher. An exact case with equal temperature and density in both codes still has to be performed.

6.7 Conclusion

The amount of particles in circular geometry is conserved, probably due to symmetry of the solution, so that the derivative of the reflective boundary condition is less important than in the simulations in X-point geometry. In X-point geometry a substantial amount of particles is lost (10%-20% depending on the resolution), which is caused by lack of application of the derivative along the plasma boundary (in this case at the divertor targets) of the reflective boundary condition. The neutral penetration depth, also known as e-folding length, is similar to the theoretical prediction. The neutral profile in JOREK has a similar shape as a run performed in EDGE2D and
Figure 6.13: As opposed to the expectation of a slight temperature drop towards the divertor targets a slight rise in temperature is observed. The cause of this faulty result has probably been discovered and is due the fact that certain temperature terms were added to the wrong position in the solution matrix.

Figure 6.14: Due to ionisation of reflected neutrals a slight rise in density towards the divertor targets is observed. The steady state solution is shown.

due to the fact that the plasma density in the EDGE2D run is 3 times higher the e-folding length is also expected to be 3 times higher, which is indeed observed. The expected drop in temperature towards the divertor targets is not observed, which is probably caused by positioning certain terms of the temperature equation in the wrong position in the solution matrix. The expected rise in density due to ionisation of reflected neutrals is observed. Increasing grid resolution improves accuracy of the solution. Improvement of the application of the derivative of the boundary condition and performing a simulation with accurate positioning of the added temperature equation terms in the solution matrix will have to be compared to a comparison case of a specialised 2D-divertor code under similar conditions (similar $T$ and similar $\rho$) and similar geometry to finally validate the code.
Chapter 7

Simulation of an ELM

7.1 Steady-state equilibrium solution

Before the plasma is allowed to destabilize as described in the next section an equilibrium solution is obtained. A steady state solution is obtained by beginning with certain initial conditions and evolving the solution for about 1 million timesteps (1 time step is 1 Alfvén time). Due to long computational times evolving the solution for several thousand timesteps is usually satisfactory. Plasma particles flowing out of the plasma are reflected as atomic neutrals and are subsequently ionised. An equilibrium is set up between the creation of neutrals through recombination and reflection at the walls and the annihilation of neutrals through ionisation. In Figure 7.1 the density profile, neutral density profile and temperature profile of the equilibrium solution is shown. The normalised values are scaled with an axis density of $n = 10^{21}$, see Appendix A for a conversion of the used scaling.

7.2 ELM Simulations

ELMs are simulated by starting from an unstable equilibrium where the stability limits of medium-n ideal ballooning modes are slightly crossed [HC07]. Inside the separatrix the edge pedestal is characterised by a large pressure gradient in the initial equilibrium. A local reduction in thermal and particle diffusivities ($D_{\text{pedestal}} = 0.1D_\perp$ and $K_{\text{pedestal}} = 0.1K_\perp$) for $\psi/\psi_{\text{separatrix}} > 0.9$ maintains the pressure gradient. The evolution of the magnetic and kinetic energies of the medium-n ballooning modes show the growth of the instability which will eventually result in total destabilisation of the plasma where an expulsion of energy and particles results from the edge of the plasma. The MHD instabilities are usually a relatively small magnetic perturbation to a large equilibrium field which is calculated in steady state. In a toroidally symmetric tokamak the toroidal mode number is a quantum number so that for small perturbations the evolution of each toroidal harmonic can be performed independently from the other harmonics. When the instabilities are small the interaction between the harmonics are small and the evolution of the system is determined by the interaction of each toroidal mode with the $n = 0$ equilibrium mode.

7.3 Simulation of an ELM in JOREK

Due to long evaluation times the simulations begin from an unstable initial condition where the stability threshold of medium-n ideal MHD ballooning modes has just been crossed. Due to the finite resistivity a significant flow in the poloidal plane is caused [HC07]. After obtaining a
Figure 7.1: Equilibrium solution of plasma density, neutral density and plasma temperature that forms a basis for simulation of the Edge Localized Mode. In the divertor region a significant amount of the particles are neutrals (up to 10%). The shown values are normalised to an axis density of \( n = 10^{21} \) and can be converted using the scaling given in Appendix A.

A satisfactory steady-state equilibrium solution the solution is perturbed with higher order harmonics which allows the plasma to become unstable.

The ELM simulation with the implemented neutral fluid model evolves well to a certain point, but eventually instability of the neutral fluid occurs at the outer divertor target. This is probably due to the incomplete application of the reflective boundary condition. This will have to be confirmed in a future run where this is problem is corrected. An old version of JOREK was used that resulted in the need for working in a low grid resolution (working in a higher resolution resulted in very high computation times, the present highest usable resolution is A=32, B=72, C=21, D=11, E=9, see Chapter 4 for an explanation of the numbers). The evolving solution is pictured in Figure 7.2.
7.4 Energy loads at divertor targets

Total energy deposited on the divertor targets can be expressed in the following formula:

\[
\Gamma_E = \Gamma_D \left[ E_B + \gamma_e T_{de} + \gamma_i T_{di} + M_D^2 (T_{de} + T_{di})/2 \right]
\]  \hspace{1cm} (7.1)

where \(\Gamma_D\) is the particle flux, \(E_B \approx 14.1\text{eV}\) is the ion binding energy released when the ion recombines at the plate, \(\gamma_e \approx 4.5\) is the electron thermal energy coefficient, \(\gamma_i \approx 2.5\) is the ion thermal energy coefficient and \(M_D = \frac{v_{\parallel}}{c}\) is the Mach Number.

After a full ELM cycle is simulated a detailed heat-load deposition profile as a function of time can be generated.
Figure 7.2: Simulation of an Edge Localized Mode. The neutral density at the divertor targets is approximately 10% of the plasma density. As the Edge Localized Mode evolves at a certain point the neutral density becomes unstable at the divertor targets. This is likely due to the incomplete application of the reflective boundary condition. This will have to be confirmed by correcting this problem.
Massive Gas Injection

Massive gas injection may be used as a method to mitigate disruptions. In Tore Supra experiments have been performed where large amounts of cold gas were injected and it was observed that the neutral gas front didn’t penetrate the plasma further than the $q = 2$ surface (stopping anywhere between $q = 2$ and $q = 2.5$). This might occur by the triggering of large radial energy transport that prevents the neutrals from penetrating deeper until a disruption occurs [RBSL*09]. Due to the injection of cold neutrals the temperature decreases significantly and the cold temperature front moves further into the plasma. The lowered temperature results in an increasing resistivity and therefore a lower current density. The disruption is highly likely destabilized by the high current density gradient (so-called tearing mode). In the experiments performed in Tore Supra [RBSL*09] a cold front of Helium particles was moving at a speed of 120 m/s. With the addition of the neutral fluid equation it is possible to simulate massive gas injection experiments and possibly reproduce the effects observed in the Tore Supra experiments. Initial simulations are performed, in a future stage simulations will have to be compared directly to experimental observations.

8.1 Simulation Setup, Assumptions and Parameters

- In a circular toroidal Tokamak setup a large amount of neutral gas is injected from the side. Since no momentum equation is added the neutrals can only transport themselves diffusively through the plasma where they are eventually ionised.

- The physical diffusion speed is much slower than the physical injection speed. Diffusion can, therefore, be ignored. This is a very crude assumption and is only legitimate for very high densities or very low temperatures, but suffices for this simulation, because a large amount of cold gas is injected both raising the density and lowering the temperature.

- The flux in a certain direction is given by $\Gamma = \rho_n v_n - D_n \frac{\partial \rho_n}{\partial r}$. Since no momentum equation is implemented for the neutrals the neutral flux has to be modelled diffusively by equating the corresponding fluxes in the horizontal direction. In the simulations the fluid speed in the horizontal direction is modelled by a high diffusion coefficient in the horizontal direction and a very low diffusion coefficient in the vertical direction.

- A linear decrease of the plasma neutral density is assumed over a characteristic distance of the plasma radius. This way the neutral diffusion coefficient can be estimated by $D_n = \frac{\rho_n v_n}{v_n R} \approx v_n R$ where $R$ is the plasma radius. With a plasma radius of $R = 1m$ and an injection speed of $v_n = 100m/s$ this amounts to a diffusion coefficient of $D_n = 100 \frac{m^2}{s}$. With a plasma
density at the the axis of $10^{20}/m^3$ this gives a normalized diffusion coefficient in the horizontal direction of $\tilde{D}_{nx} = \sqrt{\mu_0 \rho_0 D_n} = 6.482 \cdot 10^{-17} \sqrt{\mu_0 D_n} = 6.482 \cdot 10^{-7} D_n = 6.482 \cdot 10^{-5} \approx 1 \cdot 10^{-4}$. Much lower diffusion coefficients in the vertical direction and toroidal direction are employed ($\tilde{D}_{ny} = \tilde{D}_{np} = 10^{-6}$).

• Anomalous plasma diffusion coefficients and heat conduction coefficients of $D = \kappa \approx 1 m^2/s$ are chosen corresponding to normalized coefficients of $\tilde{D} = \tilde{\kappa}_\perp \approx 1 \cdot 10^{-6}$.

• The simulations are run for 3050 Alfvén times with timesteps of $\Delta t = 10\tau_{Alfvén}$.

• The total amount of injected gas in 3050 Alfvén times is about 2 times ($3 \cdot 10^{22}$ particles) the gas initially present ($1.43 \cdot 10^{22}$ particles).

8.2 Simulation results

In the following figures simulation results are shown. In Figure 8.1 the density profile over time is shown where the color shows the neutral density of the picture.

Figure 8.1: Density profile colored by the neutral density at various times during the simulation

Neutrals are injected at a high rate which are quickly ionised, resulting in a substantial decrease in temperature (Figure 8.2).

This temperature decrease results in a lowered resistivity and therefore lower current density (Figure 8.3).

In Figure 8.4 the growth of the magnetic and kinetic energy of the $n = 1$ perturbation are pictured. The steady growth of the perturbed energies eventually results in the disruption of the plasma.
In Figure 8.5 the equilibrium solution of the magnetic flux surfaces at \( t = 3050 \tau_{\text{Alfven}} \) is given showing a nested structure (note that this only the equilibrium solution, the total solution is found by addition of the \( n = 0 \) and \( n = 1 \) fluxes).

Figure 8.6 shows the \( n = 1 \) perturbation of the magnetic flux surfaces. Addition of the perturbation to the equilibrium solution is highly likely to give magnetic islands when magnetic field lines are followed and a Poincare plot is made. The magnetic islands are produced due to the tearing of the magnetic field by the onset of the tearing-mode instability.

### 8.3 Conclusion

First simulation results to reproduce the effects observed in Tore Supra experiments are very encouraging. Strong cooling after a substantial injection of particles is observed which causes the cold front to move further into the plasma. The change in temperature causes the resistivity to change, which causes large current gradients to develop. The large current gradients causes the tearing-mode MHD instability to grow which eventually results in a disruption. The next step is to compare simulations directly to experiment.
Figure 8.3: Current profile colored by the pressure profile at various times during the simulation.
Figure 8.4: Magnetic and kinetic energy of the $n = 0$ (equilibrium) and $n = 1$ solution.

Figure 8.5: Equilibrium solution of the magnetic flux surfaces.
Figure 8.6: $n = 1$ perturbation of the magnetic flux surfaces.
Summary and Conclusion

The neutral fluid equation where neutrals transport themselves diffusively through the plasma is successfully implemented in the code. Comparing the shape of the neutral density profile with an EDGE2D JET Shot gives a similar shape and the neutral penetration depth matches theoretical predictions. The JET Shot employs a different geometry than JOREK, so another comparison case in similar geometry under similar conditions (same $\rho$ and same $T$ at divertor targets) still has to be performed. The solution in JOREK is generated at grid points, where values of every variable as well as its cross-derivative and derivatives in both directions along the elements are evaluated. Visualisation of the inward flux shows proper application of the reflective boundary condition at the grid points. However, due to presence of higher order terms in the calculation of the derivative of the reflective boundary condition, the derivative of the boundary condition along the divertor targets and the rest of the wall has not been applied. This leads to small spikes in the inward neutral flux, that results in a substantial loss fraction of particles (10%-30% of the outward flux depending on the grid resolution). Working with boundary integrals as necessary in the weak form of the fluid equations in the finite element method or applying the boundary conditions in between grid points will likely solve this problem. Due to ionisation of reflected neutrals an increase in plasma density towards the divertor targets is expected, which is indeed observed. Due to consumed energy during ionisation events a slight decrease in pressure and a decrease in temperature is expected. A temperature rise near the divertor targets is, however, observed. The cause of this problem has likely been found and is due to wrong positioning of certain temperature equation terms in the solution matrix. This has been corrected and a future run will have to confirm this assumption. The code is stable in finding a steady-state solution and shows a neutral density of approximately 10% of the plasma density at the divertor targets. This can be used as an initial setup to simulate an Edge Localized Mode. The first stage of the ELM-cycle has been successfully simulated. After evolving the solution for approximately 1000 Alfvén times the neutral density solution becomes unstable at the boundary of the outer divertor target. A future run in higher resolution with correct positioning of the temperature terms in the solution matrix and correct application of the derivative of the reflective boundary condition is likely to give a better result, which is currently about to be conducted, but due to parallelisation problems has not yet been performed. After this the effects of the neutral fluid model on the fine structure of the temperature and density profile and the $D_\alpha$-emissitivity can be investigated. As a next step in improvement of the divertor region a separate temperature equation with realistic parallel conductivity coefficients (Spitzer-Harm like) can be implemented. These effects have already been implemented in JOREK and can now be integrated with the implementation of the neutral fluid model. This will allow simulation of the so-called conduction limited regime and when effects for impurities are included detached divertor regimes can also be simulated.

Additional applications for the implementation of the neutral fluid model are massive gas injection
and pellet injection. Massive gas injection simulations can now be performed with JOREK and a
massive gas injection simulation in circular geometry has been conducted resulting in a disruption as
also observed in experiments in Tore Supra. First results are extremely encouraging and reproduce
the cooling and destabilisation of the tearing-mode MHD instability. Future runs can be linked
directly to experimental observations.
Bibliography


Appendix A

Tables of Normalized Values of Parameters

A.1 Normalized values of the diffusion coefficient

The unit of the diffusion coefficient $D$ is $1\text{m}^2/\text{s}$. Normalizing the value to the JOREK code happens by multiplying the value by $\sqrt{\mathit{m}u_0\rho_0}$ which is equal to $6.482\cdot10^{-17}\sqrt{\mathit{m}_0}$ and has units of $\text{kg}/(\text{m}\cdot\text{s}\cdot\text{A})$.

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A.2 Normalized values of the temperature

The pressure $p$ equals $nk_B T = nm_D \frac{k_B T}{m_D} = \rho \frac{k_B T}{m_D}$. In JOREK the pressure is defined as a product of the mass density and a redefined temperature $\tilde{T}$ where $\tilde{T} = \frac{k_B T}{m_D}$, with units $\text{J}/\text{kg}$, so that $p = \rho \tilde{T}$.
Multiplying the temperature $\hat{T}$ by $m u_0 \rho_0 = 4.202 \cdot 10^{-33} n_0 \hat{T}$ gives the normalized temperature $\tilde{T}$:

$$\tilde{T} = 4.202 \cdot 10^{-33} n_0 \hat{T} = A \cdot \hat{T}$$

(A.1)

Hier nog de andere conversies invoegen ($\hat{T}$, $T(K)$, $\hat{T}(eV)$)

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<td>5.025 $\cdot$ 10^{-1}</td>
<td>5.025 $\cdot$ 10^0</td>
</tr>
<tr>
<td>5 $\cdot$ 10^4</td>
<td>5.8022 $\cdot$ 10^8</td>
<td>2.395 $\cdot$ 10^{17}</td>
<td>2.013 $\cdot$ 10^{-1}</td>
<td>1.005 $\cdot$ 10^0</td>
<td>1.005 $\cdot$ 10^1</td>
</tr>
<tr>
<td>1 $\cdot$ 10^5</td>
<td>1.1604 $\cdot$ 10^9</td>
<td>4.790 $\cdot$ 10^{18}</td>
<td>4.026 $\cdot$ 10^{-1}</td>
<td>2.01 $\cdot$ 10^0</td>
<td>2.01 $\cdot$ 10^1</td>
</tr>
</tbody>
</table>

Table A.2: Normalized Values of the Diffusion Coefficient
Appendix B

Code Listing

Ionisation source term and neutral diffusion coefficient

\[
\begin{align*}
sc1 &= 3.9d-1 \\
sc2 &= 2.32d-1 \\
sc3 &= 6.1d-1 \\
sc4 &= 1.5d0 \\
isourcecon1 &= 8.701d12 \\
isourcecon2 &= axisparticledensity*2.738d-24 \\
isourceconnorm &= axisparticledensity**sc4 * 2.168d-43 \\
Si0 &= sourcemultiplier*isourceconnorm*isourcecon1*(isourcecon2/T0)**(sc1)*exp(-isourcecon2/T0)/(sc2+isourcecon2/T0) \\
Si0_T &= sourcemultiplier * isourceconnorm * isourcecon1 * isourcecon2/T0**2/(0.232+isourcecon2/T0)*exp(-isourcecon2/T0)& *isourcecon2*sc1/T0**sc1*( &
& 1/(0.232+isourcecon2/T0)+1-sc1*T0/isourcecon2 ) \\
ionizationenergy0 &= ionizationenergy*axisparticledensity \\
ionizationenergy0_rh0 &= 0 \\
ionizationenergy0_T &= 0 \\
DnDOF &= 3.d0 \\
DnA &= 2.3798d32 * DnDOF/(axisparticledensity)**2 \\
DnB &= 4.116d-14 \\
DnC &= 1.209d-26*(axisparticledensity)**1.1 \\
DnD &= 8.738d23axisparticledensity \\
DnE &= 2.91d-14 \\
DnF &= 2.32d-1 \\
DnG &= 2.373d-24axisparticledensity \\
DnH &= 6.47d-17*sqrt(axisparticledensity) \\
DnJ &= 1.593d-10*axisparticledensity**(-0.15) \\
Dn0 &= DnA*DnH*(DnF*T0+DnG)/r0/(DnJ*(DnF+DnG/T0))*exp(-DnC/T0**1.1)**& T0**(0.15)+DnEx/(DnF/T0)**(0.39)*exp(-DnE/T0)) \\
Dn0_r &= DnA*DnH*(DnF*T0+DnG)/r0*(DnJ*(DnF+DnG/T0))*exp(-DnC/T0**1.1)**& T0**(0.15)+DnEx/(DnF/T0)**(0.39)*exp(-DnE/T0)) \\
Dn0_T &= DnA*DnH/DnH*(DnJ*(DnF+DnG/T0))/exp(-DnC/T0**1.1)*& T0**(0.15)+DnEx/(DnF/T0)**(0.39)*exp(-DnE/T0)) - & DnA*DnH*(DnF*T0+DnG)/r0*(DnJ*(DnF+DnG/T0))&* exp(-DnC/T0**1.1)**T0**(0.15)-DnEx& (DnF/T0)**(0.39)*exp(-DnE/T0))**2 & & ( & \\
& -DnJ*DnEx*exp(-DnC/T0**1.1)/T0**(1.85))** & \\
& 1.1*DnJ*(DnF+DnG/T0)*DnEx*exp(-DnC/T0**1.1)/T0**1.95 + & \\
& 0.15*DnJ*(DnF+DnG/T0)*exp(-DnC/T0**1.1)/T0**0.85 & \\
& -0.39*DnEx*exp(-DnE/T0)*DnJ*(DnF+DnG/T0)**0.61/T0**2 + & \\
& DnEx*(DnF/T0)**0.39*DnEx*exp(-DnE/T0)/T0**2 ) \\
\end{align*}
\]

Reflective boundary condition at divertor targets

if ((node_list%node(inode)%boundary .eq. 1) .or. (node_list%node(inode)%boundary .eq. 3)) then
if ((index_node .eq. index_min) .and. (index_node .eq. index_max)) then
   call locate_irn_jcn(index_node, index_node, index_min, index_max, ijk_position)
end if
call locate_irn_jcn(index_node,index_node2,index_min,index_max,ijA_position2)
call locate_irn_jcn(index_node,index_node3,index_min,index_max,ijA_position3)
call locate_irn_jcn(index_node,index_node4,index_min,index_max,ijA_position4)

index_large_i = n_tor * n_var * (index_node - 1)
kpsi = 1
krho = 5
KT = 6
kv = 7
krhon = 8

ilarge_rhonv = ijA_position - 1 + ((krhon-1)*n_tor + in-1) &
* n_var*n_tor + (kv-1)*n_tor + in
ilarge_rhonrho = ijA_position - 1 + ((krhon-1)*n_tor + in-1) &
* n_var*n_tor + (krho-1)*n_tor + in
ilarge_rhonpsis = ijA_position2 - 1 + ((krhon-1)*n_tor + in-1) &
* n_var*n_tor + (kpsi-1)*n_tor + in
ilarge_rhonrhont = ijA_position3 - 1 + ((krhon-1)*n_tor + in-1) &
* n_var*n_tor + (krhon-1)*n_tor + in
ilarge_rhonrhons = ijA_position2 - 1 + ((krhon-1)*n_tor+in-1)*&
* n_var*n_tor + (krhon-1)*n_tor + in
ilarge_rhonrhot = ijA_position3 - 1 + ((krhon-1)*n_tor+in-1)*&
* n_var*n_tor + (krho-1)*n_tor + in

ntnt = +1/xjac**2*(Z_s*Z_s+R_s*R_s)
nsnt = -1/xjac**2*(Z_s*Z_t+R_s*R_t)

irn_glob(ilarge_rhonv) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
jcn_glob(ilarge_rhonv) = n_tor * n_var * (index_node-1) + (kv-1)*n_tor + in
A_glob(ilarge_rhonv) = +zbig/(xjac*BigR)*r0*ps0_s/sqrt(ntnt)

irn_glob(ilarge_rhonT) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
jcn_glob(ilarge_rhonT) = n_tor * n_var * (index_node-1) + (kT-1)*n_tor + in
A_glob(ilarge_rhonT) = +zbig/sqrt(ntnt)*(Dn0_T*rn0_s*nsnt+Dn0_T*rn0_t*ntnt)

irn_glob(ilarge_rhonrho) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
jcn_glob(ilarge_rhonrho) = n_tor * n_var * (index_node-1) + (krho-1)*n_tor + in
A_glob(ilarge_rhonrho) = +zbig/sqrt(ntnt)*(1/(xjac*BigR)*Vpar0*ps0_s+rn0_t*Dn0_r*ntnt+rn0_s*Dn0_r*nsnt)

irn_glob(ilarge_rhonrhont) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
jcn_glob(ilarge_rhonrhont) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
A_glob(ilarge_rhonrhont) = + zbig*ntnt*Dn0/sqrt(ntnt)

irn_glob(ilarge_rhonrhons) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
jcn_glob(ilarge_rhonrhons) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
A_glob(ilarge_rhonrhons) = + zbig*ntnt*D_prof/sqrt(ntnt)

RHS_glob(n_tor*n_var * (index_node-1) + (krhon-1)*n_tor + in) = &
Zbig * (-1/(xjac*BigR)*r0*Vpar0*ps0_s-Dn0*rn0_s*nsnt-Dn0*rn0_t*ntnt- &
D_prof0*0.3*ntnt-D_prof0*0.3*ntnt)/sqrt(ntnt)

endif
dendif
Reflective Boundary Condition Wall Aligned With Fluxsurface

if ((index_node .ge. index_min) .and. (index_node .le. index_max)) then
  call locate_irn_jcn(index_node,index_node, index_min,index_max,ijA_position)
  call locate_irn_jcn(index_node,index_node2,index_min,index_max,ijA_position2)
  call locate_irn_jcn(index_node,index_node3,index_min,index_max,ijA_position3)
  index_large_i = n_tor * n_var * (index_node - 1)
  ilarge_rhonrhos = ijA_position2 - 1 + ((krhon-1)*n_tor+in-1)*n_var*n_tor+(krho-1)*n_tor+in
  ilarge_rhonrhot = ijA_position3 - 1 + ((krhon-1)*n_tor+in-1)*n_var*n_tor+(krho-1)*n_tor+in
  ilarge_rhonrhons = ijA_position2 - 1 + ((krhon-1)*n_tor+in-1)*n_var*n_tor+(krhon-1)*n_tor+in
  ilarge_rhonrhont = ijA_position3 - 1 + ((krhon-1)*n_tor+in-1)*n_var*n_tor+(krhon-1)*n_tor+in
  nsns = -1/xjac**2*(Z_t*Z_t+R_t*R_t)
  nsnt = -1/xjac**2*(Z_s*Z_t+R_s*R_t)
  irn_glob(ilarge_rhonrhos) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonrhos) = n_tor * n_var * (index_node2-1) + (krho-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonrhos) = Aglob(ilarge_rhonrhos)+zbig*nsns*D_prof/sqrt(nsns)
  else
    A_glob(ilarge_rhonrhos) = +zbig*nsns*D_prof/sqrt(nsns)
  endif
  irn_glob(ilarge_rhonrhot) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonrhot) = n_tor * n_var * (index_node3-1) + (krho-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonrhot) = Aglob(ilarge_rhonrhot)+zbig*nsnt*D_prof/sqrt(nsns)
  else
    A_glob(ilarge_rhonrhot) = +zbig*nsnt*D_prof/sqrt(nsns)
  endif
  irn_glob(ilarge_rhonrho) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonrho) = n_tor * n_var * (index_node-1) + (krho-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonrho) = Aglob(ilarge_rhonrho) +zbig*(nsns*Dn0_r*rn0_s+rn0_t*nsnt*Dn0_T)/sqrt(nsns)
  else
    A_glob(ilarge_rhonrho) = +zbig*(nsns*Dn0_r*rn0_s+rn0_t*nsnt*Dn0_T)/sqrt(nsns)
  endif
  irn_glob(ilarge_rhonT) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonT) = n_tor * n_var * (index_node-1) + (kT-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonT) = Aglob(ilarge_rhonT)+zbig*(nsns*Dn0_T*rn0_s+rn0_t*nsnt*Dn0_T)/sqrt(nsns)
  else
    A_glob(ilarge_rhonT) = +zbig*(nsns*Dn0_T*rn0_s+rn0_t*nsnt*Dn0_T)/sqrt(nsns)
  endif
  irn_glob(ilarge_rhonrhos) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonrhos) = n_tor * n_var * (index_node3-1) + (krho-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonrhos) = Aglob(ilarge_rhonrhos)+zbig*nsns*0/sqrt(nsns)
  else
    A_glob(ilarge_rhonrhos) = +zbig*nsns*0/sqrt(nsns)
  endif
  irn_glob(ilarge_rhonrhont) = n_tor * n_var * (index_node-1) + (krhon-1)*n_tor + in
  jcn_glob(ilarge_rhonrhont) = n_tor * n_var * (index_node3-1) + (krhon-1)*n_tor + in
  if ((node_list%node(inode)%boundary .eq. 3)) then
    A_glob(ilarge_rhonrhont) = Aglob(ilarge_rhonrhont)+zbig*nsnt*0/sqrt(nsns)
  else
    A_glob(ilarge_rhonrhont) = +zbig*nsnt*0/sqrt(nsns)
  endif
  if ((node_list%node(inode)%boundary .eq. 3)) then
    RHS_glob(n_tor*n_var * (index_node-1) + (krhon-1)*n_tor + in) = &
    RHS_glob(n_tor*n_var * (index_node-1) + (krho-1)*n_tor + in) = &
    -zbig*D_prof*r0_s*nsns/sqrt(nsns)-zbig*nsnt*D_prof*r0_t/sqrt(nsns)
    -zbig*Dn0*nsns*rn0_s/sqrt(nsns)-zbig*Dn0*nsnt*rn0_t/sqrt(nsns)
  else
    RHS_glob(n_tor*n_var * (index_node-1) + (krhon-1)*n_tor + in) = &
    -zbig*D_prof*r0_s*nsns/sqrt(nsns)-zbig*D_prof*r0_t/sqrt(nsns)
    -zbig*Dn0*nsns*rn0_s/sqrt(nsns)-zbig*Dn0*nsnt*rn0_t/sqrt(nsns)
  endif
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Additional boundary condition at corner points

! This boundary condition has to be included when the density is fixed
! at the boundaries parallel to the flux surfaces.
! This prevents numerical instability of the corner points in this case.
! When the plasma density is variable at the boundary parallel
! to the flux surfaces this boundary condition does not need to be applied.

if ((node_list%node(inode)%boundary .eq. 31)) then

  T0 = node_list%node(inode)%values(1,1,6)
  r0 = node_list%node(inode)%values(1,1,5)
  Dn0 = DnA*DnH*(DnF*T0+DnG)/r0/(DnJ*(DnF+DnG/T0)**exp(-DnC/T0**1.1)) &
    *exp(-(DnF/T0**1.1)*T0**((0.15)+DnE*(DnG/T0)**0.39)*exp(-DnG/T0))
  Dn0_r = -DnA*DnH*(DnF*T0+DnG)/r0**2/(DnJ*(DnF+DnG/T0)** &
    exp(-DnF/T0**1.1)*T0**((0.15)+DnE*(DnG/T0)**0.39)*exp(-DnG/T0))
  Dn0_T = DnA*DnH*DnF/r0/(DnJ*(DnF+DnG/T0)** &
    exp(-DnF/T0**1.1)*T0**((0.15)+DnE*(DnG/T0)**0.39)*exp(-DnG/T0)) - &
    DnA*DnH*(DnF*T0+DnG)/r0/(DnJ*(DnF+DnG/T0)** &
    exp(-DnF/T0**1.1)*T0**((0.15)+DnE*(DnG/T0)**0.39)*exp(-DnG/T0))**2* &
    ( -DnJ*DnG*exp(-DnC/T0**1.1)/T0**(1.85)+1.1*DnJ*(DnF+DnG/T0)*DnC*exp(-DnC/T0**1.1)/T0**1.95 + &
      0.15*DnJ*(DnF+DnG/T0)*exp(-DnF/T0**1.1)*T0**(1.85)+1.1*DnJ*(DnF+DnG/T0)**0.39*DnG/ &
      T0**2 )
  ps0 = node_list%node(inode)%values(1,1,1)
  psi_dif = abs(ps0)-abs(psi_bnd)
  D_prof = D_perp(1) * ((1.0-D_perp(2)) + D_perp(2) **&
    (0.500 - 0.500*tanh((psi_norm-D_perp(5)) /D_perp(4))))
  Vpar0 = node_list%node(inode)%values(1,1,7)
  Vpar0_s = node_list%node(inode)%values(1,2,7)
  Vpar0_t = node_list%node(inode)%values(1,3,7)
  ps0_s = node_list%node(inode)%values(1,2,1)
  ps0_t = node_list%node(inode)%values(1,3,1)
  R = node_list%node(inode)%x(1,1)
  R_s = node_list%node(inode)%x(2,1)
  R_t = node_list%node(inode)%x(3,1)
  Z = node_list%node(inode)%x(1,2)
  Z_s = node_list%node(inode)%x(2,2)
  Z_t = node_list%node(inode)%x(3,2)
  r0_s = node_list%node(inode)%values(1,2,8)
  r0_t = node_list%node(inode)%values(1,3,8)
  r0_st = node_list%node(inode)%values(1,4,8)
  r0 = node_list%node(inode)%values(1,1,5)
  r0_s = node_list%node(inode)%values(1,2,5)
  r0_t = node_list%node(inode)%values(1,3,5)
  r0_st = node_list%node(inode)%values(1,4,5)
  xjac = R_s*Z_t - R_t*Z_s
  index_node = node_list%node(inode)%index(1)
  index_node2 = node_list%node(inode)%index(2)
  index_node3 = node_list%node(inode)%index(3)
  index_node4 = node_list%node(inode)%index(4)
  nsns = +1/xjac**2*(Z_t*Z_t+R_t*R_t)
  nsnt = -1/xjac**2*(Z_s*Z_t+R_s*R_t)
  ntnt = +1/xjac**2*(Z_s*Z_s+R_s*R_s)
  outflux = D_prof*r0_s*nsns+D_prof*r0_t*nsnt
  influx = Dn0*r0_s*nsns*Dn0*r0_t*nsnt
  ! write(*,*) 'R: ', R, 'Z: ', Z

endif
endif
A-Matrix and RHS plasma density equation (primarily already existing in code, added ionisation source term)

amat_51 = - (D_par-D_prof) * BigR * BB2_psi / BB2**2 * Bgrad_rho_star * Bgrad_rho * xjac * theta * tstep &
+ (D_par-D_prof) * BigR / BB2 * Bgrad_rho_star_psi * Bgrad_rho &
xjac * theta * tstep &
+ (D_par-D_prof) * BigR / BB2 * Bgrad_rho_star * Bgrad_rho_psi &
xjac * theta * tstep &
+ v * Vpar0 * (r0_s * psi_t - r0_t * psi_s) * theta * tstep &
+ v * r0 * (vpar0_s * psi_t - vpar0_t * psi_s) * theta * tstep &
RHS_glob(n_tor*n_var * (index_node3-1) + (krhon-1)*n_tor + in) = &
-zbig*(nsns-nsnt*sqrt(nsns)/sqrt(ntnt)*ooratios)
\[ rhs_{ij,5} = v \times \text{BigR} \times \text{particle\_source}(ms,mt) \times \text{tstep} + v \times \text{BigR}^{\times 2} \times (r_0_s \times u_0_t - r_0_t \times u_0_s) \times \text{tstep} + v \times 2.d0 \times (\text{GAMMA}-1.d0) \times \text{BigR} \times T_0 \times u_0_y \times \text{tstep} - \frac{\text{ZK}_\text{par}-\text{ZK}_\text{prof}}{\text{BB}_2} \times \text{Bgrad}_T^* \times \text{Bgrad}_T \times \text{tstep} - \text{zeta} \times v \times \text{r}_0 \times r_{\text{neutral}0} \times S10 \times \text{BigR} \times \text{jac} \times \text{tstep} \]

A-matrix and RHS temperature equation, added terms for particle ionisation, particle diffusion and ionisation energy losses

\[ rhs_{ij,6} = v \times \text{BigR} \times \text{heat\_source}(ms,mt) \times \text{tstep} + v \times r_0 \times \text{BigR}^{\times 2} \times (T_0_s \times u_0_t - T_0_t \times u_0_s) \times \text{tstep} + v \times r_0 \times 2.d0 \times \frac{\text{epsi}_cyl^*}{\text{BigR}^*} \times \text{BigR} \times \text{tstep} - \frac{\text{ZK}_\text{par}-\text{ZK}_\text{prof}}{\text{BB}_2} \times \text{Bgrad}_T^* \times \text{Bgrad}_T \times \text{tstep} - \text{zeta} \times v \times r_0 \times v \times \text{delta}_g(mp,6,ms,mt) \times \text{BigR} \times \text{jac} \times \text{tstep} \]

amat_61 = - (\text{ZK}_\text{par}-\text{ZK}_\text{prof}) \times \text{BigR} / \text{BB}_2 \times \text{Bgrad}_T^* \times \text{Bgrad}_T \times \text{tstep} + \frac{\text{ZK}_\text{par}-\text{ZK}_\text{prof}}{\text{BB}_2} \times \text{Bgrad}_T^*_\text{psi} \times \text{Bgrad}_T \times \text{tstep} + \frac{\text{ZK}_\text{par}-\text{ZK}_\text{prof}}{\text{BB}_2} \times \text{Bgrad}_T^* \times \text{Bgrad}_T_{\text{psi} \text{psi}} \times \text{tstep} + \frac{\text{zeta} \times v \times r_0 \times v \times \text{delta}_g(mp,6,ms,mt) \times \text{BigR} \times \text{jac} \times \text{tstep}}{\text{tstep}} \]

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amat_62 = - v * r0 * BigR**2 * ( T0_s * u_t - T0_t * u_s) &
* theta * tstep &
- v * r0 * 2.d0* (GAMMA-1.d0) * BigR * T0 * u_y &
* xjac * theta * tstep
amat_65 = - v * rho * BigR**2 * ( T0_s * u0_t - T0_t * u0_s) &
* theta * tstep &
- v * rho * 2.d0* (GAMMA-1.d0) * BigR * T0 * u0_y &
* xjac * theta * tstep &
+ v * rho * FO / BigR * Vpar0 / T0_p &
* xjac * theta * tstep &
+ v * rho * Vpar0 / ( T0_s * ps0_t - T0_t * ps0_s) &
* theta * tstep &
+ v * rho * (GAMMA-1.d0) * T0 * (vpar0_s * ps0_t - vpar0_t * ps0_s) &
* xjac * theta * tstep &
+ v * rho * BigR * rho_neutral0 * S10 * ionizationenergy0 &
* xjac * theta * tstep &
+ v * rho * BigR * rho_neutral0 * S10 * ionizationenergy0 &
* xjac * theta * tstep &
+ v * rho * BigR * rho_neutral0 * S10 &
* xjac * theta * tstep &
amat_66 = v * r0 * T * BigR &
* xjac * (1.d0 + zeta) &
- v * r0 * BigR**2 * ( T_s * u0_t - T_t * u0_s) &
* theta * tstep &
- v * r0 * 2.d0* (GAMMA-1.d0) * BigR * T * u0_y &
* xjac * theta * tstep &
+ ZK_prof * BigR * (v_x*T_x + v_y*T_y + v_p*T_p /BigR**2 ) &
* xjac * theta * tstep &
+ v * r0 * FO / BigR * Vpar0 / T0_p &
* xjac * theta * tstep &
amat_67 = + v * r0 * F0 / BigR &
* xjac * theta * tstep &
+ v * r0 * F0 / BigR &
* xjac * theta * tstep &
amat_68 = + v * r0 * FO / BigR &
* xjac * theta * tstep &
A-Matrix and RHS neutral density equation

87
amat_85 = + v * r_neutral0 * Si0 * rho * BigR * xjac * theta * tstep &
+ Dm0_y * (v_x*r_neutral0_x + v_y*r_neutral0_y + v_p*r_neutral0_p * eps_cyl**2 /BigR**2 &
)*rho*BigR*theta*xjac*tstep

amat_86 = + v * r0 * r_neutral0 * Sin_T * T * BigR * theta * xjac * tstep + &
Dn0_T * (v_x*r_neutral0_x + v_y*r_neutral0_y + v_p*r_neutral0_p * eps_cyl**2 /BigR**2 ) * T &
BigR * xjac * theta * tstep

amat_88 = v * rho_neutral * BigR * xjac &
+ Dm0*(v_x*rho_neutral_x+v_y*rho_neutral_y* &
v_p*rho_neutral_p*eps_cyl**2/BigR**2)*BigR*theta*xjac*tstep &
+ v*r0*Si0*rho_neutral*theta * BigR * xjac * tstep

rhs_ij_8 = -Dm0 * BigR * (v_x * r_neutral0_x+v_y * r_neutral0_y+v_p*r_neutral0_p*eps_cyl**2/BigR**2) &
* xjac * tstep - v * r0 * r_neutral0 * Sin * BigR * xjac * tstep &
+ v * BigR * neutral_source(as,nt) *xjac *tstep