

# **Modelling of Kinetic Effects in Parallel Transport in the Tokamak Scrape-Off Layer**

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for the degree of Doctor of Philosophy in Physics at  
Imperial College London.

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*To my parents and my wife.*

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## The role of the author

This work is part of the collaboration between Imperial College London and the Culham Centre for Fusion Energy. As such, it was performed with the input of people from both institutions, with the author's role being that of a front line software developer as well as a funnel for both their own and collaborators' ideas. The code SOL-KiT, which has resulted from this work, and as presented in this thesis, has been completely developed by the author. However, it is being contributed to and expanded by others, and it itself borrows from many approaches that have come before. Those ideas which the code has borrowed are clearly attributed to their sources in the text.

Unless otherwise stated, the data presented has been obtained and analysed by the author using SOL-KiT. All external data sources are clearly cited when the data is used. Figure reproduction permissions have been obtained where necessary.

## Declaration

I hereby declare that material used and information reported in this thesis is entirely original, unless otherwise acknowledged in the text.

**Stefan Mijin**

23/06/2020

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## Abstract

Heat flow onto divertor targets in the tokamak represents one of the main design problems in current fusion research. Excessive heat loads, especially during violent transient events, can significantly damage the plasma-facing components. In order to mitigate the heat load it is beneficial to run the tokamak in a detached regime. This involves formation of a neutral cloud in front of the divertor targets that protects the surface material. Thus interaction of the plasma with the detached neutrals becomes important.

Energy, on its way to the divertor targets, travels through the boundary region of the tokamak, the Scrape-Off Layer. The main transport direction is parallel to the open magnetic field lines of the Scrape-Off Layer. Fluid models are routinely used to simulate particle and energy transport in the boundary region, but these fail to capture kinetic effects, which have been linked to discrepancies between said fluid model predictions and experimental data[1]. Kinetic/non-local effects have been observed in simulations of parallel transport, including heat flux suppression and enhancement[2], as well as effects on ionisation rates[3]. The plasma sheath at the divertor target is also affected by non-local phenomena[4, 5]. Exploring how kinetic effects change facets of parallel transport, and especially how they cause departure from widely used fluid models, is important in furthering our understanding of heat load issues, which are critical to future machine design.

In this thesis, a novel framework for studying electron kinetic effects in parallel transport is developed, with special focus on the proper treatment of the sheath boundary condition and inelastic collisions, and the capability of self-consistent comparison between a kinetic and fluid model. This framework is implemented in the new electron kinetic code SOL-KiT, and details on the model and numerics, as well as benchmarking, are presented.

With the developed code, a systematic power scan study of non-local effects in both equilibria and transients has been conducted. Kinetic effects are found to be especially prominent in the interaction of transients with detachment, where heating due to fast particles, heat flux suppression, as well as modification of ionisation rates have been observed.

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# List of commonly used symbols

|                             |                                                                 |
|-----------------------------|-----------------------------------------------------------------|
| $A$                         | Atomic mass                                                     |
| $\vec{B}, B_\theta, B_\phi$ | Magnetic field vector and its toroidal and poloidal components  |
| $D$                         | Diffusion coefficient                                           |
| $\vec{E}, E_x$              | Electric field vector and its parallel component                |
| $F_l$                       | $l$ -th Legendre harmonic of the ion distribution function      |
| $K$                         | Knudsen number                                                  |
| $K^e, K^{ion}$              | Excitation/ionisation rate                                      |
| $L$                         | Characteristic/connection/domain length                         |
| $M$                         | Mach number, heavy particle mass                                |
| $N_t$                       | Number of timesteps                                             |
| $N_x, N_v$                  | Number of points on spatial/velocity grid                       |
| $P_l$                       | $l$ -th Legendre polynomial                                     |
| $\mathbf{P}$                | Pressure tensor                                                 |
| $Q$                         | Energy source                                                   |
| $R$                         | Major tokamak radius, friction terms                            |
| $S$                         | Particle source                                                 |
| $T_j$                       | Temperature of species $j$                                      |
| $U_e$                       | Electron internal energy density                                |
| $Z$                         | Atomic number, ion charge                                       |
| $a$                         | Minor tokamak radius, acceleration magnitude                    |
| $\vec{a}$                   | Acceleration vector                                             |
| $b$                         | Impact parameter, atomic state number                           |
| $c_s$                       | Ion sound speed                                                 |
| $f_j$                       | Distribution function of species $j$                            |
| $f_l$                       | $l$ -th Legendre harmonic of the electron distribution function |
| $g_i$                       | Quantum degeneracy of atomic state $i$                          |
| $j_e$                       | Electron current                                                |
| $l$                         | Legendre harmonic number                                        |
| $n_j$                       | Density of species $j$                                          |
| $p$                         | Isotropic pressure                                              |

|                            |                                                                  |
|----------------------------|------------------------------------------------------------------|
| $q$                        | Safety factor, heat flux, charge                                 |
| $q_{\parallel}, q_x, q_e$  | Parallel conductive (electron) heat flux                         |
| $q_{sh}$                   | Total heat flux into the sheath                                  |
| $q^{TOT}$                  | Total (conductive and convective) heat flux                      |
| $\vec{q}$                  | Conductive heat flux vector                                      |
| $\vec{r}$                  | Radius vector                                                    |
| $t$                        | Time                                                             |
| $\vec{u}_j$                | Flow velocity vector of species $j$                              |
| $v_n$                      | Position of $n$ -th point on velocity grid                       |
| $v_{\parallel}, v_{\perp}$ | Parallel/perpendicular velocity (with respect to magnetic field) |
| $v_{th}$                   | Electron thermal speed                                           |
| $\vec{v}$                  | Velocity vector                                                  |
| $x$                        | Position along the magnetic field - $x$ -axis                    |
| $x_k$                      | Position of $k$ -th point on spatial grid                        |

### Greek Symbols

|                 |                                                                        |
|-----------------|------------------------------------------------------------------------|
| $\Delta t$      | Timestep length                                                        |
| $\Delta v_n$    | Width of $n$ -th velocity cell                                         |
| $\Delta x_k$    | Width of $k$ -th spatial cell                                          |
| $\Gamma_j$      | Particle flux of species $j$                                           |
| $\Gamma_{sh}$   | Particle flux into the sheath                                          |
| $\ln \Lambda$   | Coulomb logarithm                                                      |
| $\Omega$        | Solid angle                                                            |
| $\alpha_b$      | Three-body recombination rate for neutral state $b$                    |
| $\alpha_s$      | Heat flux limiter for species $s$                                      |
| $\beta_b$       | Radiative recombination rate for neutral state $b$                     |
| $\Delta\Phi$    | Sheath potential drop                                                  |
| $d\sigma$       | Differential cross-section                                             |
| $\epsilon$      | Inelastic collision energy loss, atomic transition energy              |
| $\gamma$        | Sheath heat transmission coefficient                                   |
| $\kappa$        | Heat conductivity                                                      |
| $\lambda_D$     | Debye length                                                           |
| $\lambda_{ss'}$ | Collisional mean free path for collisions between species $s$ and $s'$ |
| $\mu$           | Reduced mass                                                           |
| $\nu^*$         | Upstream SOL collisionality                                            |
| $\omega_p$      | Plasma frequency                                                       |
| $\varphi$       | Azimuthal angle                                                        |
| $\sigma$        | Differential or integral cross-section                                 |

|                |                                                                    |
|----------------|--------------------------------------------------------------------|
| $\sigma^{TOT}$ | Integral cross-section                                             |
| $\tau_E$       | Energy confinement time                                            |
| $\tau_e$       | Characteristic electron collision time                             |
| $\tau_{SOL}$   | Acoustic transition time along the SOL                             |
| $\theta$       | Deflection angle, angle between velocity vector and magnetic field |

### Physical Constants

|              |                          |                                                                           |
|--------------|--------------------------|---------------------------------------------------------------------------|
| $a_0$        | Bohr radius              | $5.291772109 \times 10^{-11} \text{ m}$                                   |
| $c$          | Speed of light in vacuum | $299,792,458 \text{ m/s}$                                                 |
| $e$          | Electron charge          | $1.60217662 \times 10^{-19} \text{ C}$                                    |
| $h$          | Plank Constant           | $6.62607 \times 10^{-34} \text{ Js}$                                      |
| $k$          | Boltzmann Constant       | $1.38064852 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$ |
| $m_e$        | Electron mass            | $9.10938356 \times 10^{-31} \text{ kg}$                                   |
| $m_p$        | Proton mass              | $1.6726219 \times 10^{-27} \text{ kg}$                                    |
| $\epsilon_0$ | Vacuum permittivity      | $8.8541878 \times 10^{-12} \text{ F/m}$                                   |

# Chapter 1

## Introduction

### 1.1 Thermonuclear fusion and the Tokamak

Before delving into the intricacies of electron transport in the Scrape-Off Layer, it is important to motivate this narrow and deep investigation, lest the forest be lost for the trees. As humanity is faced with the challenge of powering an increasingly demanding society, while concerns for the environment grow, new methods of energy production become desirable. Depletion of oil and natural gas reserves is inevitable, predicted to happen within this century, while coal reserves will last for a few more centuries [6]. One could also (and in the author's opinion *should*) argue that the environmental impact of energy production must be a prime concern in the development of future power grids. While steps have been taken to switch to renewable energy sources, these increased efforts have so far produced some expensive failures [7], and humanity's continued reliance on fossil fuels is easily gleaned from the maps produced at [www.electricitymap.org](http://www.electricitymap.org) (see Figure 1.1). Although low-carbon (see France in Figure 1.1), nuclear fission produces great quantities of highly dangerous waste, the disposal of which has become a great concern. Considering all of these points, the development of a (mostly) clean source of reliable energy with practically limitless fuel would go a long way to ensuring that our future society is both powered and sustainable. Thermonuclear fusion could well be that source, and in this section both the basic principles of a general fusion reactor, as well as the specific reactor design of the tokamak will be introduced in order to provide a basic platform for the study to follow.

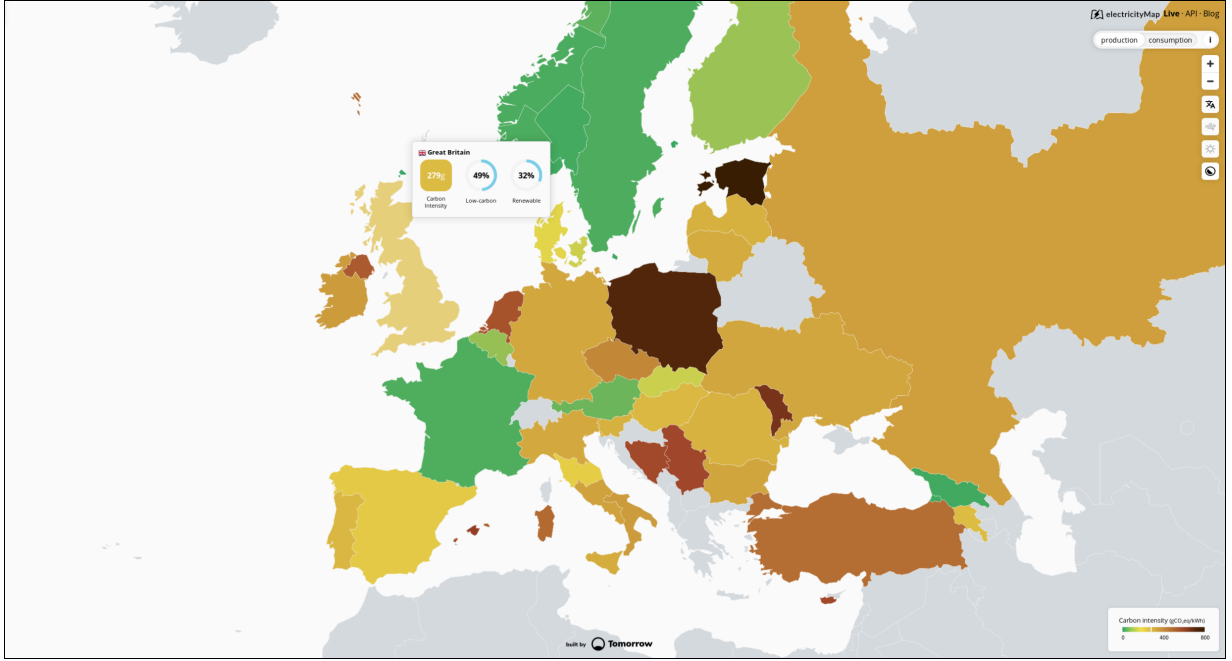


Figure 1.1: CO<sub>2</sub> emission map of Europe due to electricity production. Taken from [www.electricitymap.org](http://www.electricitymap.org) at 13:33 GMT on July 30th 2019.

### 1.1.1 Thermonuclear fusion

The basic energy producing reaction in a fusion power plant would be that of deuterium-tritium (D-T) fusion. This reaction produces an alpha particle and a neutron, and has been deemed the most promising candidate out of the several deuterium fusion reactions. In D-T fusion



the 17.6MW of energy is split between the  $\alpha$ -particle (3.5MW) and the neutron (14.1MW). Figure 1.2 shows the cross-section of this reaction, as well as those of the other widely considered deuterium reactions. It can be seen that the dominant reaction (in terms of cross-section) is indeed D-T fusion.

While Figure 1.2 shows a peak in the D-T cross-section at 100keV, the necessary temperatures in a fusion core of a reactor would be much less. Assuming the reactants are thermalised, their velocity distribution is Maxwellian

$$f_j(v) = n_j \left( \frac{m_j}{2\pi kT} \right)^{3/2} \exp \frac{-m_j v^2}{2kT}, \quad (1.2)$$

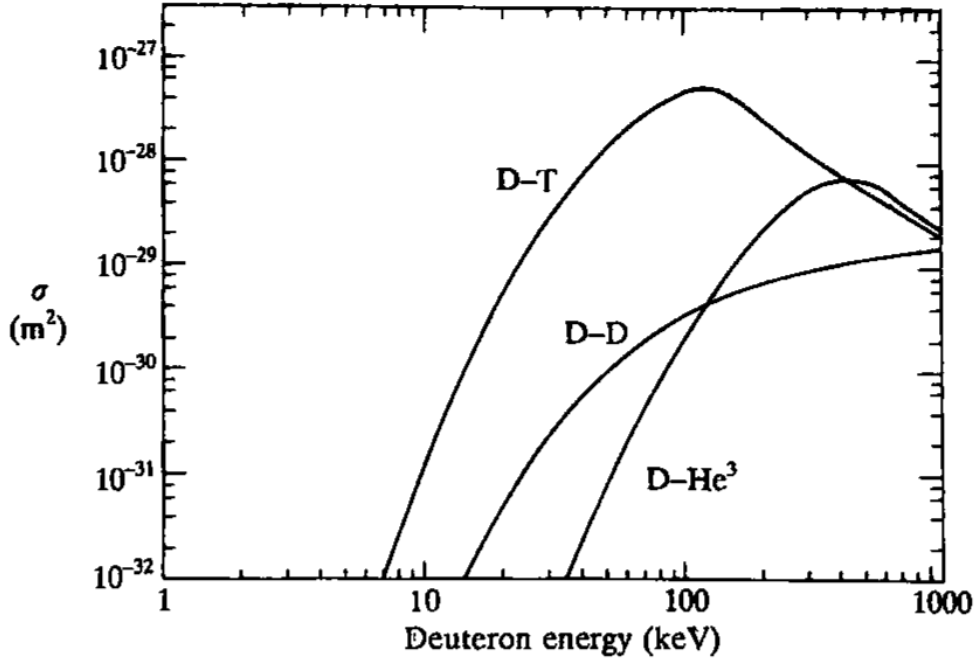


Figure 1.2: Cross-sections for the nuclear fusion reactions of D-T, D-D, and D-He<sup>3</sup>. Taken from [8].

where  $n_j$  and  $m_j$  are the density and atomic mass of species  $j$ , respectively, and  $T$  is the temperature (assuming all species are at the same temperature). The reacting particles are then those in the distribution tail, and the relevant temperatures for a reactor are of the order of 10 keV. At these temperatures, the fusion fuel is fully ionised, i.e. it is a plasma. The total energy contained in the plasma is then  $W = 3nkTV$ , with  $n$  being the total density of particles (deuterium and tritium), and  $V$  the volume of the reactor core. The factor of 3 comes from the fact that both electrons and ions contribute  $3nkT/2$  to the energy density. Temperature and density are assumed constant for simplicity.

An important concept in fusion research and reactor design is that of ignition[8]. Much in the same vein as internal combustion engines, once the fuel is ignited, the reactor operates with no input (heating) power  $P_H$ , instead maintaining fusion conditions with power obtained from the fusion reaction itself. This power comes in the form of alpha heating  $P_\alpha$ , as the  $\alpha$ -particles deposit their share of the reaction energy (a fifth) into the plasma, while the neutrons escape the fusion core without much in the way of interaction. If the energy loss rate is labeled as  $P_L$ , the ignition condition would then be  $P_\alpha \geq P_L$ . In case of simple flat profiles of density and

temperature,  $n$  and  $T$  respectively, and with energy confinement time defined as  $\tau_E = W/P_H$ , it can be shown that the ignition criterion [9] is given by

$$nT\tau_E \geq 3 \times 10^{21} \text{m}^{-3} \text{keVs}. \quad (1.3)$$

In other words, a sufficiently dense and hot plasma needs to be confined for a long enough time for it to ignite. For example, the above condition would be reached in a plasma with  $T = 10 \text{keV}$ ,  $n = 10^{20} \text{m}^{-3}$ , and  $\tau_E = 3 \text{s}$ . Of course, the criterion is different for plasmas of different shape, but these numbers give a general idea of reactor conditions.

Another major concept in general fusion reactor design is the so-called Q-factor, the ratio of fusion power (a fifth of which is given to the  $\alpha$ -particles) to heating power

$$Q = \frac{5P_\alpha}{P_H}. \quad (1.4)$$

Thus the Q-factor indicates how close to ignition the plasma is, with  $Q$  going to infinity at ignition. While the perk of ignition is that no extra power needs to be added into the system, a  $Q$  value that is high enough would still provide viable reactor conditions, albeit at the cost of some of the produced power being fed back into the reactor core. As such, reactor design becomes a chase of ever higher values of  $Q$ .

### 1.1.2 The Tokamak

The tokamak is a toroidal magnetically-confined fusion (MCF) device [8]. In order to have a stably confined plasma in a torus, two components of the magnetic field are necessary. These are illustrated in Figure 1.3. The toroidal component  $B_\phi$ , as the name suggests, runs along the torus, and is produced by magnetic coils outside the vacuum vessel that contains the plasma. In order to produce the poloidal field  $B_\theta$ , a toroidal current must be induced. The current necessary to produce sufficiently strong poloidal fields is of the order of 10MA, with those fields generally an order of magnitude weaker than the toroidal fields, which are on the order of several T in modern tokamaks. The resulting field winds around the torus, and is shaped using additional coils. Magnetic field lines inside the core form closed nested toroidal surfaces, referred to as

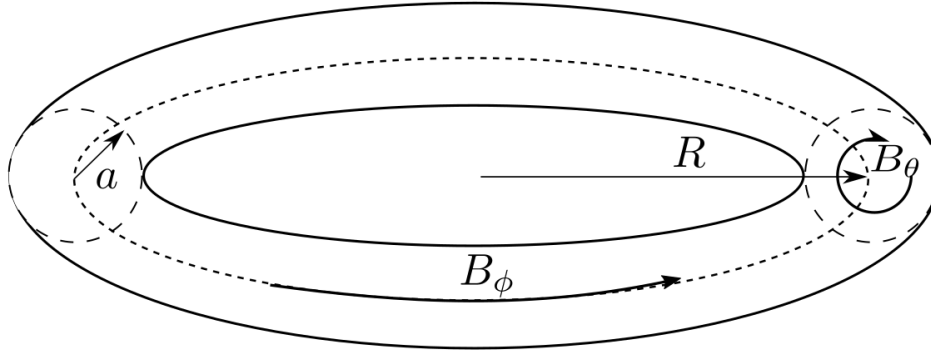


Figure 1.3: Simple scheme of magnetic fields in a tokamak. Toroidal  $B_\phi$  and poloidal  $B_\theta$  fields together confine the plasma. The minor and major radii of the tokamak,  $a$  and  $R$  respectively, are shown.

flux surfaces. Each flux surface can be labeled with its own minor radius  $r \leq a$ . In realistic situations, these surfaces are shaped, and the flux surface label becomes more complicated than just  $r$ , although still unique for each surface[10].

A reactor tokamak would have further components, such as the radiation shield, as well as the lithium blanket, used to capture neutron energy as heat, and breed tritium for fuel [8, 11]. The details of conceptual reactor design are beyond this text, and only those aspects that influence the physics investigation that follows will be focused on.

As was noted above when discussing the basic concepts, there will always be losses. In other words, confinement is not perfect, and this fact is a double-edged sword. On the one hand, good confinement is necessary for power production (see equation (1.3)). On the other hand, perfect confinement would also confine  $\alpha$ -particles that have already transferred their energy to the plasma. This is referred to as helium ash, and its accumulation leads to the quenching of the fusion reaction. Thus it is established that the escape of energy and particles from the core is both inevitable, and, to an extent, necessary. This raises several questions, chief of which are "Where do the escaped energy and particles go?" and "What are the possible mechanisms of this escape?". Answers to both of these questions, and more, lie in the physics of the plasma boundary layer, the region outside of the hot core.

## 1.2 Basics of exhaust physics

The short answer to the first of the two questions is that energy and particles are ejected into the boundary region of the reactor, where they find their way to the plasma facing components (PFCs) of the reactor[12]. The term plasma exhaust is frequently used for the processes involved in extracting energy and particles through the boundary region, known also as the Scrape-Off Layer (SOL). A myriad of physical aspects is important in the area of exhaust physics. In this section, the important exhaust processes will be reviewed briefly so as to provide a basis for the complications touched upon in the following section.

The SOL will be discussed in detail in the next chapter, when the physics basis of the study presented in this thesis is introduced. However, several important points are needed to motivate the upcoming discussion. Firstly, as opposed to the closed helical magnetic field lines of the core pictured schematically in Figure 1.3, the boundary region is characterised by open field lines impinging on material surfaces. Due to the dynamics of the plasma, the transport parallel to those lines is vastly different to the cross-field transport, the main difference being the disparate time scales of the transport in the two directions. As will be illustrated in the next chapter, the transport in the parallel direction is much faster. Another difference between the two directions is that of the main transport mechanisms. While the parallel direction hosts conductive and convective transport, cross-field transport is dominated by anomalous diffusion and turbulent structures, such as blobs/filaments[13]. Magnetic field geometry also plays an important role in both parallel and perpendicular transport.

In either direction, the plasma will interact with atomic and molecular neutrals and impurity ions, whose parallel and cross-field transport is as important as that of the plasma leaving the core. The plasma and the neutrals interact with the material surfaces, causing erosion, and, depending on the surface chemistry, can produce a wide range of interactions that influence transport[14]. Furthermore, a desirable operating regime called detachment (covered in more detail in the next chapter) gives great importance to the interaction of the plasma with the neutrals, as it involves a cloud of neutral particles providing a buffer between the plasma and the PFCs. Thus, the veritable “soup” of interactions involving various neutral and impurity

species can carry great weight in determining the physics of the plasma exhaust.

The second question posed above, about the mechanisms of escape, is decidedly more difficult to answer, primarily because of the fact that many of these mechanisms are yet to be properly described. Broadly speaking, one can categorise the transport out of the core as either steady state or transient transport. Steady state transport will always be present, while transient events can have many causes, but the main ones would be instabilities of the core, such as Edge-Localised Modes (ELMs). Filaments are another transient effect important in transporting particles and energy out of the core. These two types of transients are very different, especially as they manifest in different operating regimes, with filaments manifesting in both low and high confinement modes, while ELMs are present only in regimes of high confinement.

Whatever the mechanism of escape might be, the energy ejected into the SOL travels towards the material surfaces, and represents the heat load on those plasma-facing surfaces. It is exactly this heat load that has been identified as one of the most important factors in the design and operation of future reactors[15]. For example, ITER projections predict that the maximum deposited power flux at the divertor target (the main PFC, discussed in the next chapter) to be on the order of several tens of  $\text{MW}/\text{m}^2$ , while uncontrolled ELMs in ITER are predicted to deliver energy fluxes around  $20\text{MJ}/\text{m}^2$ , comparable to energy fluxes experienced by shuttles on re-entry[16].

While cross-field transport of both the plasma and, especially, the neutrals is important for a complete understanding of the plasma exhaust, the focus of this thesis is on the parallel component of transport. Due to it being much faster than perpendicular transport, it plays the main role in determining heat flow to the divertor, but can also couple with cross-field transport, for example through filament temperature decay rates[17]. The parallel direction can experience extreme gradients in temperature and density, especially during transients. Combined with the plasma-neutral interactions, the strong collisionality gradients can distort distribution functions, and produce non-local effects, which are the topic of this thesis and discussed below.

### 1.3 The problem of non-locality

Modelling of SOL transport, such as that used to provide heat load projection on ITER, is usually performed using a fluid description of the plasma. A major assumption in such fluid models is that of locality. This amounts to treating plasmas with  $L \gg \lambda$ , where  $L$  is the plasma length scale (determined by the physical size, as well as various gradients), while  $\lambda$  is the relevant collision mean free path. In other words, high enough collisionality must be assumed in order to treat a plasma as a fluid. In these cases the distribution functions of the plasma species are very close to Maxwellian, and the treatment of the small deviations from that form produces various fluid models (e.g. Braginskii [18]). A non-local plasma thus has species with distribution functions deviating significantly from a Maxwellian. Hereafter the terms non-local and non-Maxwellian will be used interchangeably, focusing on the non-local effects produced by such distributions and ignoring the subtler meanings of the terms.

In the SOL, due to the presence of strong gradients along the field line, the distribution functions of all species in the plasma are likely non-local. A more detailed discussion on non-locality in the SOL will be given in the form of a literature review at the end of the following chapter. At this point, however, it should be noted that it was suggested that non-local effects can explain discrepancies between fluid modeling and experimental observations in the SOL[1], and non-local effects have been observed in multiple models.

In general, non-locality can impact a wide range of problems in the SOL, including, but not limited to [19]:

- Plasma transport - including the transport of particles, energy, as well as that of neutrals and impurities[20, 21, 22, 23],
- Plasma-surface interactions - including non-isotropic recycling, impurity sputtering, etc.[24],
- Transient phenomena - such as Edge-Localised Modes (ELMs), filamentary structures, gas puffs, etc.[13, 25, 17, 26, 27, 28],
- Interpretation of diagnostics - including spectroscopic and probe data.[29, 30, 31]

In order to properly account for non-local effects, the distribution function must be modelled using a kinetic approach. Ideally, one would have detailed accounts of both the electron and ion distribution properties throughout the SOL. Attempts have been made to simulate both ions and electrons kinetically[2, 4], and non-local effects have been observed in both the plasma species as well as the neutrals. These effects include spatially varying suppression of heat flux compared to the expected fluid value, rapidly rising heat flow due to fast particles not captured by a fluid model, as well as ionisation and erosion rate modification. However, as will be discussed in detail in the next chapter, these simulations can be extremely computationally expensive. This means that a simpler model must serve as a starting point for any investigation, regardless of long-term goals. The main objective of the work behind this thesis was in laying the groundwork for systematic long-term fundamental exploration of kinetic effects in the SOL, and thus electron kinetics is tackled first. Developing a framework for the study of the electron kinetic effects during transients was one of the major goals. As the interaction of transients with detachment is an important current research concern, understanding how electron kinetics affect this interaction is necessary for future reactor design choices. Furthermore, the general coupling of electrons and neutral species in the SOL through various inelastic processes and how that coupling is changed due to electron kinetic effects is an area that could benefit from more research. Thus the goal of this study can be summarised as: “Develop and utilise a kinetic electron model to highlight and study non-local effects during equilibria and transients, especially in the context of transient-detachment interaction”. The structure of the thesis is described below.

## 1.4 Thesis structure

The remainder of the thesis is structured as follows, with the intent to provide a flowing account of the work performed.

**Chapter 2:** The Scrape-Off Layer (SOL), as the boundary region of MCF devices, is introduced. The different configurations and physical regimes are covered, with a focus on simplified models and phenomenological descriptions. Given that the study is focused on kinetic effects in the

SOL, a short introduction to kinetic theory is presented, followed by a brief overview of the important atomic and molecular effects in the SOL. Finally, the chapter is concluded with a review of selected results from the literature, aimed at rounding out and focusing the discussion for the specialised chapters ahead.

**Chapter 3:** Analytical aspects of the model developed for implementation in the new code SOL-KiT is presented, with a focus on novel and important features. Both the fluid and kinetic models used for the electrons are given, with the Legendre polynomial formalism used in the kinetic approach. The extensive suite of collisional operators used in the study is introduced here, before concluding with the first description of the important material surface boundary condition in terms of Legendre polynomials.

**Chapter 4:** The introduction of SOL-KiT is continued with the numerical aspects of the model. Normalisation, discretisation, and algorithms used to solve the resulting matrix equation are discussed. Special attention is given to the conservative discretisation of inelastic electron-neutral collision operators, with it being derived and the associated grid mappings discussed in detail. Benchmarking tests performed with SOL-KiT are presented to verify that the code is operating as expected. The contents of this chapter and the previous one have been submitted to Computer Physics Communications[32].

**Chapter 5:** Both equilibrium and transients simulations were the focus of the first study performed using SOL-KiT. In this chapter, the kinetic SOL equilibria resulting from an input power scan are analysed and compared to corresponding fluid equilibria in order to identify kinetic effects. The differences in detachment behaviour between fluid and kinetic models are presented, before moving on to transient simulations, where the domination of kinetic effects is demonstrated. The results of this chapter have been accepted for publishing[33].

**Chapter 6:** Electron energy transport channels are analysed for the simulations performed in the previous chapter. Non-local effects are found in both the general behaviour of channels, associated to different detachment onsets, as well as in individual channels. Heating due to fast

particles, as well as effects of heat flux suppression are presented and discussed. Finally, the kinetic effects on atomic rates are discussed. Contents of this chapter are part of a paper in preparation[34].

**Chapter 7:** The presented results are summarised, with the main conclusions of the previous two chapters emphasised. Limitations of the current model are noted, before concluding on the potential future studies possible with the framework developed for this thesis.

# Chapter 2

## Physics basis

### 2.1 Overview

In the previous chapter the tokamak was introduced in simple terms, with the focus on the energy and particles escaping the core and threatening the material surfaces through transport. Due to its vast complexity and the interplay of physical and chemical processes, the physics of the boundary region through which this transport occurs has been labeled “kitchen” physics[10]. The interaction of the plasma with surfaces and various atomic and molecular impurities is the primary source of this (derogatory) label, as it differs greatly from the analytically tractable fully ionised ideal plasmas. The full range of boundary plasma physics is well beyond the scope of this text, and this chapter shall focus on introducing those terms and tools necessary for the study of kinetic electron transport that follows.

The next section shall introduce the basic terms and models used to understand the Scrape-Off Layer and its various regimes. An introduction to collisional kinetic theory terms and equations follows, providing the main tool of the presented investigation. Atomic and molecular effects due to hydrogen are briefly discussed, merely skimming the surface of the “kitchen” physics. Focus is then shifted on a selection of previous studies of non-local effects in the Scrape-Off Layer, with the aim of concisely rounding out the discussion and equipping the reader with the very basic understanding of general approaches as well as certain expectations of what non-local effects manifest as in the plasma boundary layer.

## 2.2 The Scrape-Off Layer

In this section the boundary region of MCF devices, the Scrape-Off Layer (SOL), is introduced. Before tackling the two main configurations of the SOL, it is important to give an overview of plasma-surface interactions and the basics of the plasma sheath. Once the role of solid surfaces as plasma sinks is established, the simplified magnetic field geometry and the characteristic physical quantities important in the SOL are presented. A simple model of energy flow based on the classical result of Spitzer-Härm rounds out the introduction to the SOL, and lays down groundwork for the complications of kinetic theory.

### 2.2.1 Plasma-wall interaction and the sheath

Steady state fluid flows are induced through the existence of local sources and sinks of particles. In a plasma, the sources are provided by the ionisation of atoms and molecules, while recombination acts as a sink. Atomic physics of hydrogenic plasmas will be explored later, but it is necessary to note the two types of recombination at this point - volume and surface recombination. When plasma comes into contact with a solid surface, ions impinging onto it pick up electrons from the surface and are returned into the plasma as neutral particles. This is surface recombination, also referred to as plasma recycling[35] in SOL physics. Recycling acts as the main plasma sink in the SOL, inducing flows.

Another important aspect of plasma-surface interaction is that of the plasma sheath. When a solid surface is immersed in a low temperature plasma, such as that in the SOL, it becomes charged negatively due to the higher mobility of electrons compared to that of ions (positive charging is possible in some corner cases, but will be ignored in this treatment). A region of positive charge then forms close to the surface, screening the negative charge on the wall. This region is referred to as the plasma sheath[36, 37, 38].

The formation of the plasma sheath is the manifestation of a fundamental property of plasmas, i.e. the tendency to maintain quasineutrality[36, 37]. Quasineutrality in a plasma with electrons and ions of charge  $Ze$  simply means that  $n_e \approx Zn_i$ , where  $n_e$  and  $n_i$  are electron and ion densities, respectively. One can think of quasineutrality as the simple fact that plasmas act

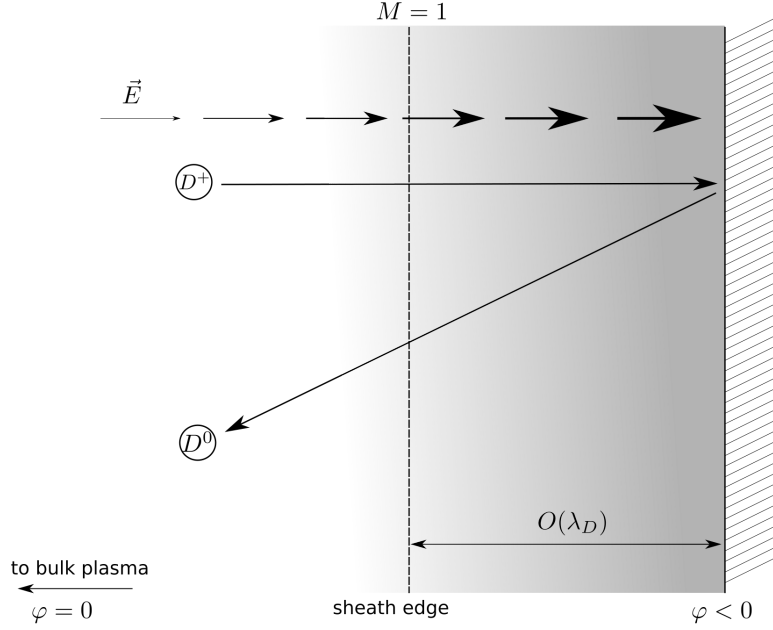


Figure 2.1: The most important aspects of plasma-surface interaction - plasma sheath formation and recycling.

to counteract the effects of external electric fields. This is why a thin region of positive spatial charge forms near a negatively charged surface. The spatial extent of the plasma sheath is given by a basic plasma scale length - the Debye length  $\lambda_D$ , which for a two-component plasma has the form

$$\frac{1}{\lambda_D} = \sqrt{\frac{n_e e^2}{\epsilon_0 k T_e} + \frac{n_i Z^2 e^2}{\epsilon_0 k T_i}}, \quad (2.1)$$

where  $T_e$  and  $T_i$  are the electron and ion temperature. For plasma conditions in the SOL, the Debye length is the shortest length scale of interest .

A large potential drop forms on a scale of several Debye lengths near a surface. The resulting electric field accelerates ions, and it can be shown that in order to avoid discontinuities in the solution, the ion flow velocity  $u_i$  must satisfy the Bohm criterion at the sheath edge [38, 12]

$$u_i \geq c_s \approx \sqrt{\frac{k(\gamma_e^p T_e + \gamma_i^p T_i)}{m_i}}, \quad (2.2)$$

where  $c_s$  is the ion sound speed, with  $m_i$  being the ion mass. This is also sometimes stated as ions reaching Mach number  $M = u_i/c_s$  of 1. The two dimensionless numbers,  $\gamma_e^p$  and  $\gamma_i^p$ ,

represent the electron and ion polytropic coefficients. In the remainder of this text, both will be assumed to be unity (although they can, in principle, change to accommodate different sound speed assumptions).

An important concept for the study of boundary plasmas is that of the sheath potential drop  $\Delta\Phi$ . Usually, the potential at the surface is more negative due to the greater mobility of electrons compared to ions. A simple way to estimate  $\Delta\Phi$  is by assuming that the wall charges until thermal electrons can no longer reach it, giving the energy balance  $e\Delta\Phi \approx kT_e$ , leading to the potential drop being  $\Delta\Phi = O(kT_e/e)$ .

Another important aspect of plasma-surface interaction is that of sputtering[39, 40, 41, 12]. Sputtering is the erosion and subsequent release of the surface material into the plasma. The main type of sputtering in a hydrogenic plasma in contact with metal is physical sputtering via ion impact. While not treated in the presented work, it is important to mention as it is the main source of impurities in a tokamak, and their transport through the SOL and into the core is associated with a decrease of fusion power, and in some cases even violent disruptions of the discharge.

To summarise, the role of plasma-surface interactions in a reactor plasma is both that of a plasma sink, as well as the source of neutral particles. As these particles travel away from the surface, they are ionised, and thus present a source of plasma. The sink action of the surface induces flows, and these flows reach the ion sound speed close to the surface - on a scale of several Debye lengths. The plasma can be considered quasineutral away from this sheath edge, with quasineutrality breaking down on the Debye scale. Figure 2.1 shows a summary of the most important properties of the sheath and plasma-surface interaction.

### 2.2.2 The limiter SOL and general SOL properties

The simplest configuration of the Scrape-Off Layer is the limiter configuration[12]. The aim is to limit the extent of the core by opening the magnetic field lines. This is achieved, in the limiter case, by protruding wall segments. A JET (Joint European Torus) plasma in limiter configuration is shown in Figure 2.2. The toroidal axis is perpendicular to the paper. As the limiter is along the toroidal axis, this configuration is referred to as a toroidal limiter. The

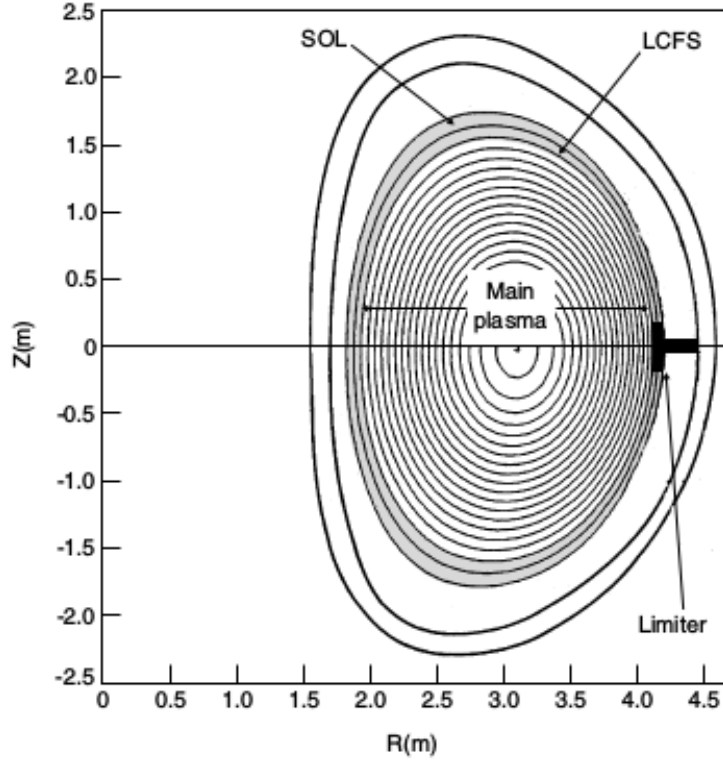


Figure 2.2: The limiter configuration in a JET-like plasma. Poloidal cross-section shown, toroidal axis perpendicular to paper. The SOL is shown in grey. Taken from [12].

last flux surface in the main plasma is referred to as the last closed flux surface (LCFS). The Scrape-Off Layer is then the entire extent of the plasma beyond the LCFS.

It is informative to revisit the magnetic geometry in order to define several important terms relating to the SOL. For this purpose, a flat torus projection of a flux surface is shown in Figure 2.3. The axes show the toroidal and poloidal circumference. The magnetic field lines are labeled  $\vec{B}_{TOT}$ , and the angle they make with the toroidal direction, the pitch angle  $\theta$ , is given by

$$\theta = \arctan \frac{B_\theta}{B_\phi}, \quad (2.3)$$

which for small pitch angle (the usual case) simplifies to  $\theta = B_\theta/B_\phi$ . It is then possible to define the safety factor  $q$  as the number of toroidal turns a field line makes before making one poloidal turn. In the case of the field line in Figure 2.3  $q = 3$ . If an imaginary toroidal limiter is then inserted at some poloidal position in the figure (which implies  $r = a$ ), the connection length  $L$  can be defined as the length of the magnetic field line between two intersections with the limiter. For a small pitch angle (relatively large  $q$ ), this is approximated by

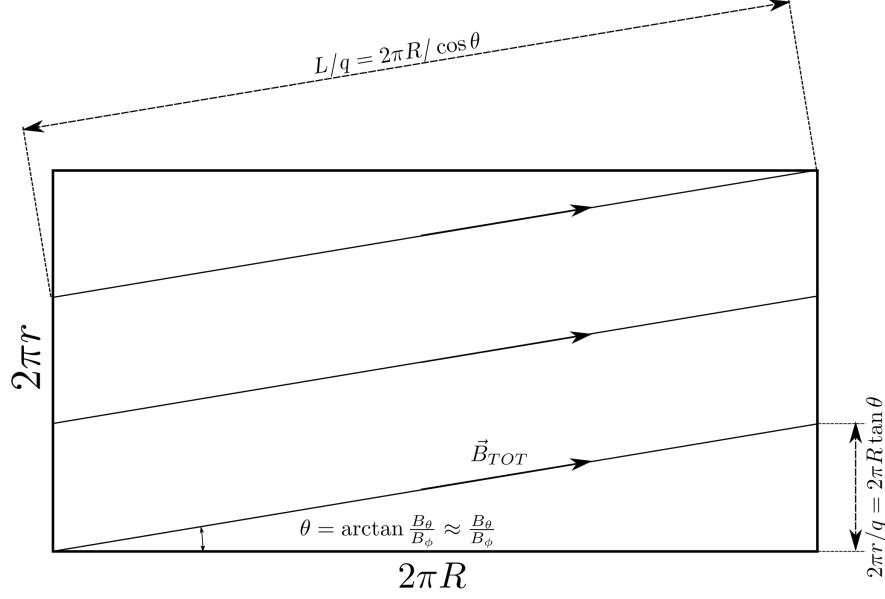


Figure 2.3: Flat torus projection of a  $q = 3$  magnetic surface, showing the pitch angle  $\theta$  and defining the connection length  $L$ . Bottom axis shows circumference along toroidal direction, while the left axis gives poloidal circumference.

$$L \approx 2\pi Rq, \quad (2.4)$$

where a general expression for the safety factor is given by

$$q = \frac{rB_\phi}{RB_\theta}. \quad (2.5)$$

Thus the parallel extent of the SOL, the connection length  $L$ , is defined. What about its extent perpendicular to the magnetic field, i.e. in the radial direction? For this purpose, the two competing transport directions in the SOL[12] must be considered. As noted in the previous section, the characteristic velocities in the parallel direction are on the scale of the ion sound speed  $c_s$ . In order to treat the perpendicular direction, Fick's law of diffusion is used. While the diffusive transport in the SOL is anomalous, the rough estimate of the perpendicular velocity given by diffusion is enough in order to infer the SOL width. The diffusive approximation gives for the perpendicular velocity

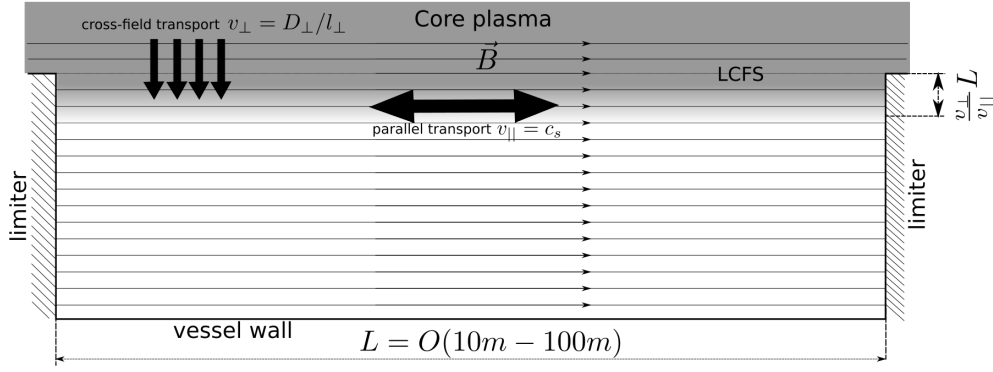


Figure 2.4: Formation of the thin SOL as determined by the competition of parallel and perpendicular transport.

$$v_{\perp} = \frac{D_{\perp}}{l_{\perp}}, \quad (2.6)$$

where  $D_{\perp}$  is taken from experiment (of the order of  $1\text{m}^2/\text{s}$ ). For the characteristic density gradient length  $l_{\perp}$  the ionisation mean free path can be used. This then gives for  $v_{\perp}$  values of order  $1\text{m/s}$ . The perpendicular extent of the SOL,  $Lv_{\perp}/c_s$ , is then much shorter than the connection length  $L$ , owing to the ion sound speed being around four orders of magnitude greater than  $v_{\perp}$ . The competition between perpendicular and parallel transport in a limiter configuration is pictured in Figure 2.4. Note that in this approach the SOL has been straightened out, getting rid of the curvature effects in the magnetic field. Such an approach is standard in the analysis of SOL transport, especially when dealing mainly with the parallel direction.

The characteristic time scale of parallel particle transport in the SOL can be written as

$$\tau_{\text{SOL}} = \frac{L}{c_s}. \quad (2.7)$$

In the following sections and chapters the various processes in the SOL will be explored, with differing time and length scales. While the main topic will be collisional processes, one must also keep in mind the timescales of energy and density perturbations in the SOL, and how these compare with  $\tau_{\text{SOL}}$ . Furthermore, the ratio of the characteristic length scales of various collisional processes (the mean free paths) and the connection length  $L$  will inform the choice of model, and acts as a parameter defining different regimes.

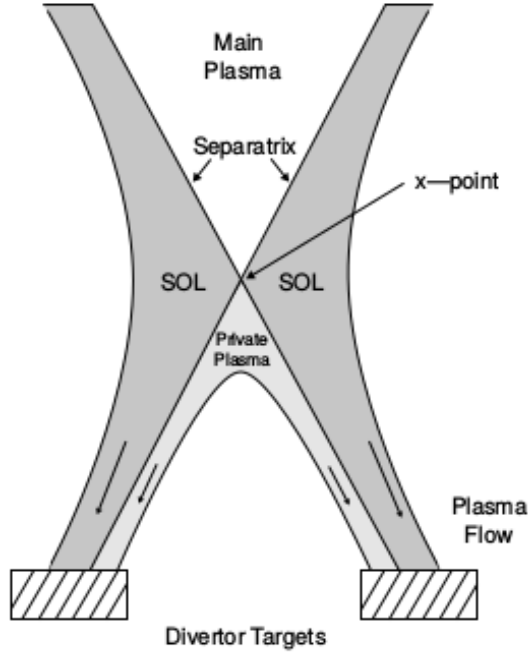


Figure 2.5: The divertor SOL and its main features. LCFS is replaced by the separatrix, and the geometry is further complicated by the existence of the X-point. Taken from [12].

### 2.2.3 The divertor SOL and the Two-Point Model

The second SOL configuration, and the one this work focuses on, is the so-called divertor configuration. Instead of opening the magnetic field lines by inserting what is, effectively, a metal rod, one can opt instead to install secondary coils, which would shape the magnetic field and produce the open field lines characteristic to the SOL. A simplified schematic of the divertor SOL is shown in Figure 2.5.

The anatomy of a divertor configuration is more complicated than in the limiter case. This is primarily due to the magnetic field geometry, specifically the existence of the X-point, which is located on the separatrix (the divertor analogue to the limiter LCFS), the imaginary line separating the three main plasma regions in the divertor configuration. At the X-point, the poloidal component of the magnetic field vanishes, and the region around the X-point experiences particularly strong magnetic shear effects, heavily distorting plasma flows and structures that pass through it. In Figure 2.5 the three main plasma regions are shown. When compared to the limiter case where only two regions are visible (the main plasma and SOL), the divertor configuration has the addition of the private plasma region, into which plasma is transported

via perpendicular transport from the SOL. The SOL can be further separated into the region above the X-point, and the region below it, referred to as the divertor region. As the name implies, the divertor configuration diverts plasma flows onto specifically designed surfaces - the divertor targets.

The divertor has a number of advantages compared to the limiter. The first of these is rather obvious, and is the larger separation between the plasma core and the main plasma facing component, the targets. With the plasma-surface interactions occurring farther away from the core, contamination due to sputtered impurities can be better controlled. While the surface area over which the plasma escaping the core deposits its energy (plasma-wetted area) is generally larger in the limiter case, the power loads on divertor targets can be reduced via volumetric losses in the divertor region. Operation in the divertor configuration lead to the discovery of the so-called H-mode (high confinement mode)[42], which can yield higher fusion power. A particular beneficial operating scenario, the detached regime[43, 44], is also more easily obtained in the divertor configuration. Different divertor regimes, including detachment, will be explored in the next section.

While there are many advantages of the divertor configuration, its main disadvantage is the simple fact that the magnetic volume is much larger than in the limiter case. Magnetic volume is expensive, so the divertor advantages have to outweigh the increased economic cost of inefficient use of magnetic volume. Another trade-off in operating in H-mode, as opposed to the low confinement L-mode, is the appearance of potentially devastating transients - Edge Localised Modes. These will be briefly introduced towards the end of this chapter.

In order to model the divertor SOL in the simplest way, it is again straightened out, as shown in Figure 2.6. The two ends of the system represent reference points upstream and at the target. Using just quantities at these two points it is possible to attain basic insight into the divertor SOL. Appropriately, the model describing these two points is referred to as the Two-Point Model(2PM) in the literature[12, 45]. Subscripts 'u' and 't' denote physical quantities at the two points in question.

The starting assumption is that all of the ionisation happens in a thin region near the target, and that no momentum loss or volume recombination occurs anywhere, as well as neglecting



Since any temperature change across the ionisation region is ignored, after integrating the above equation along the connection length  $L$  the second Two-Point Model equation is obtained

$$T_u^{7/2} = T_t^{7/2} + \frac{7}{2} \frac{q_{||} L}{\kappa_{0e}}. \quad (2.11)$$

Finally, a boundary condition for the heat flux at the target sheath is needed. It is possible to show that, for a Maxwellian plasma, this can be written as [12]

$$q_{||} = \gamma k T_t \Gamma_t, \quad (2.12)$$

where  $\gamma \approx 7$  is the so-called sheath heat transmission coefficient and  $\Gamma_t$  is the particle flux at the target, assuming the Bohm criterion. The sheath heat transmission coefficient contains both an electron and an ion contribution  $\gamma = \gamma_e + \gamma_i$ .

With three equations (2.9),(2.11),(2.12) and 5 unknowns (assuming  $L$  is a known parameter),  $n_u, n_t, T_u, T_t, q_{||}$ , it is necessary to choose two control parameters. The usual choices are  $n_u$  and  $q_{||}$ , as those are easily controlled experimentally, by adjusting fueling and heating. Since in equation (2.11) the temperatures are raised to a high power, even a small drop in the target temperatures renders  $T_u^{7/2} \gg T_t^{7/2}$ . This produces the following scalings for the remaining three parameters

$$T_u \propto L^{2/7} q_{||}^{7/2}, \quad (2.13)$$

$$T_t \propto n_u^{-2} L^{-4/7} q_{||}^{10/7}, \quad (2.14)$$

$$n_t \propto n_u^3 q_{||}^{-8/7} L^{6/7}. \quad (2.15)$$

Particularly important to notice is the strong density dependence in equation (2.14). A high upstream density reduces the target temperature, opening the door to regimes where the heat loads to the divertor target as well as the sputtering of impurities is mitigated. This is fortunate to the extent that a high upstream density can be associated with a higher core density, which is beneficial to fusion reaction rates. The effect of increasing density will be explored further in

depth in the next section, when different divertor regimes are introduced.

Before moving on to the discussion of divertor regimes, it is important to address some of the assumptions in the Two-Point Model and how they can be relaxed [12]. The three main assumptions that can be relaxed are the following

- No momentum loss - introducing momentum loss factor  $f_{\text{mom}}$ ,
- No volumetric power loss - introducing power loss factor  $f_{\text{power}}$ ,
- No convective heat transfer - introducing conduction factor  $f_{\text{cond}}$ .

Starting from the assumption of no momentum loss, it is relaxed by allowing friction with the neutrals, either through elastic or inelastic collisions, as well as effects such as viscosity. This is all captured in one factor, and equation (2.9) becomes

$$2n_t T_t = (1 - f_{\text{mom}})n_u T_u. \quad (2.16)$$

Some fraction of the input power can be assumed lost through radiation and charge-exchange  $q_{\text{loss}} = f_{\text{power}} q_{||}$ . This modifies equation (2.12) to

$$(1 - f_{\text{power}})q_{||} = \gamma n_t k T_t c_s. \quad (2.17)$$

Note that the assumption of a localised region of plasma-neutral interaction is not relaxed here - the power loss occurs close to the target. This allows the use of the conduction equation (2.10), but with the heat flux separated into its conductive and convective components,  $q_{||} = q_{\text{cond}} + q_{\text{conv}}$ . Assuming that the ratio of conductive and convective fluxes remains constant throughout the SOL so that  $q_{\text{cond}} = f_{\text{cond}} q_{||}$ , the updated version of equation (2.11) is

$$T_u^{7/2} = T_t^{7/2} + \frac{7}{2} \frac{f_{\text{cond}} q_{||} L}{\kappa_{0e}}. \quad (2.18)$$

Using the more general equations, (2.16), (2.18), and (2.17), one can update the scalings of  $n_t, T_t$ , and  $T_u$  to include the various loss factors.

However, the above modifications still do not change the fact that the Two-Point Model is a 0D model. The assumptions of reduced geometry, classical heat conduction, and the neglect of

cross-field transport all limit the Two-Point Model. Nonetheless, it is still an illustrative first step with a surprising amount of accuracy, and remains widely used, albeit with varying degrees of modification.

### 2.2.4 Divertor regimes

The divertor configuration allows for different regimes, and these can be characterised first by collisionality. Taking  $n_e = n_i = n$  and  $T_i = T_e = T$  similarly to the simplest Two-Point Model case, it is possible to approximate the thermal Coulomb self-collision (electron-electron or ion-ion) mean free path as [12]

$$\lambda \approx 10^{16} \frac{T^2}{n} [\text{m}], \quad (2.19)$$

with temperature expressed in eV and density in  $\text{m}^{-3}$ . A collisionality parameter based on the upstream quantities  $n_u$  and  $T_u$  and the connection length  $L$  can be defined as

$$\nu^* = \frac{L}{\lambda_u}. \quad (2.20)$$

Varying the collisionality induces transitions between the various divertor regimes. The transition points are not rigorously defined, but a simple characterisation of the different regimes is based on the ratio of upstream and downstream temperatures, which (following from the Two-Point Model) has the following dependence on collisionality [12]

$$\frac{T_u}{T_t} \propto (\nu^*)^2. \quad (2.21)$$

The three divertor regimes usually discussed are, in order of increasing collisionality

- The sheath-limited regime,
- The conduction-limited regime,
- The detached regime.

The sheath-limited regime has the smallest drops in temperature along the SOL. Pressure is constant along the flux tube, and thus plasma density remains mostly constant. This means that the target effectively experiences the same plasma conditions as those upstream, making this regime conceptually differ only slightly compared to the limiter case.

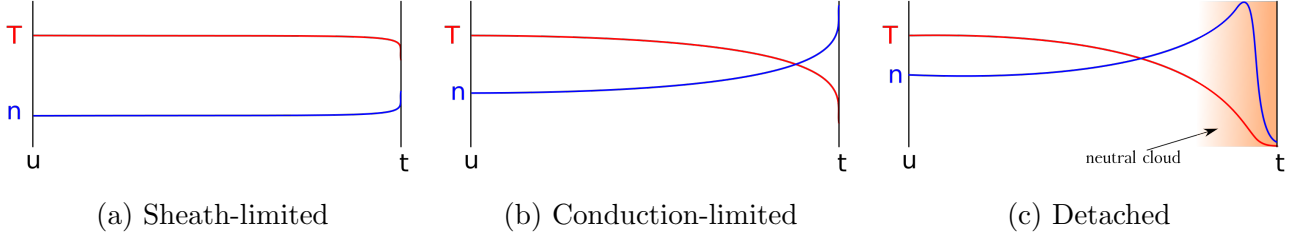


Figure 2.7: An illustration of temperature and density profiles characterising the discussed divertor regimes. Density increases from left to right.

As collisionality increases, conduction starts dominating, and the temperature gradient grows. Since pressure is still constant, the plasma density at the target rises. This leads to an accompanying increase in plasma flux onto the target surface, where it recombines. As such, the conduction-limited regime overlaps with what is referred to in the literature as the high recycling regime. Note that while the temperature drops, there is still not enough momentum loss from plasma neutral collisions to reduce pressure at the target. This means that even though the plasma ionises the neutrals produced through recycling, the particle fluxes still deliver most of this ionisation energy through electrons and ions impinging onto the surface.

If the temperature at the target continues to drop, a significant fraction of the neutrals will remain unionised. This neutral cloud (usually partially) “detaches” the target from the plasma. The resulting increase in plasma-neutral friction and volume recombination produces a drop in

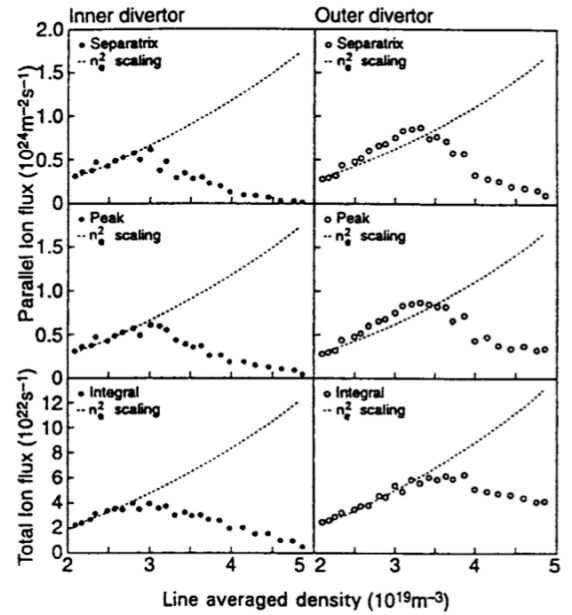


Figure 2.8: Detachment onset in JET divertor. As density increases flux rollover is observed in both divertor legs. Taken from [12].

pressure, which manifests itself as a drop in target density. Such a state is highly desirable as it would increase the lifetime of the divertor target components. As the momentum loss kicks in and reduces pressure at the target, the ion flux at the target drops. This contrasts the flux increase experienced as target temperatures drop in the conduction-limited regime.

The mentioned decrease in ion flux at the target is used as an experimental criterion for detachment onset[45]. Measuring ion saturation current with Langmuir probes, one can observe non-monotonic behaviour, a so-called “flux rollover”. Usually observed in density scans, where increasing the density effectively ramps up collisionality, one such example of rollover in the JET divertor is shown in Figure 2.8.

## 2.3 Kinetic theory basics

A plasma contains many particles, with tokamak densities in excess of  $n = 10^{20}\text{m}^{-3}$  [47, 8]. If the Hamiltonian or Lagrangian system for the motion of all  $N_0$  of the particles were to be solved this would result in  $6N_0$  or  $3N_0$  equations. Ignoring the impossibility of the task, that amount of information is not only unnecessary, but also obfuscates the important aspects of the macroscopic behaviour of our system. In order to describe the physics at a level of detail our human minds can more easily resolve, methods of statistical physics are applied to develop the kinetic equation. The next section will deal with the distribution function and the two most common ways of deriving the kinetic equation, namely the phase space formalism of the Liouville equation[48] and the BBGKY[49, 50] hierarchy, as well as the Klimontovich approach[51]. Following that, collision integrals of interest in the study presented in this work will be introduced, before finally going over the transition from kinetic to fluid formalism through the moments of the distribution function. The general approach in this section is mostly based on the books by Swanson and Bellan [52, 37].

### 2.3.1 The kinetic equation and the distribution function

The starting point in the derivation of the kinetic equation is the  $6N_0$ -dimensional phase space inhabited by a system of  $N_0$  particles. Let these particles be affected by some general force  $F$ ,

so that the equations of motion of particle  $i$  are

$$\frac{\partial \vec{V}_i}{\partial t}(t) = \vec{F}(\vec{r}_i, \vec{v}_i, t), \quad (2.22)$$

$$\frac{\partial \vec{R}_i}{\partial t}(t) = \vec{V}_i(t), \quad (2.23)$$

where  $\vec{V}_i(t)$  and  $\vec{R}_i(t)$  are the position and velocity of particle  $i$  at time  $t$ , respectively. Coordinates  $\vec{r}_i$  and  $\vec{v}_i$  are phase space coordinates in the  $6N_0$ -dimensional space. The density of particles in this phase space can be defined as follows [52]

$$N(\vec{r}_1, \vec{v}_1, \vec{r}_2, \vec{v}_2, \dots, \vec{r}_{N_0}, \vec{v}_{N_0}, t) = \prod_{i=1}^{N_0} \delta[\vec{r}_i - \vec{R}_i(t)] \delta[\vec{v}_i - \vec{V}_i(t)]. \quad (2.24)$$

The Liouville equation describes the evolution of this phase space density. Using the following property of the Dirac delta function

$$\frac{\partial}{\partial t} \delta[\vec{r}_i - \vec{R}_i(t)] = -\frac{\partial \vec{R}_i}{\partial t} \cdot \nabla_{\vec{r}_i} \delta[\vec{r}_i - \vec{R}_i(t)], \quad (2.25)$$

the Liouville equation is obtained

$$\frac{\partial N}{\partial t} + \sum_{i=1}^{N_0} \vec{V}_i \cdot \nabla_{\vec{r}_i} N + \sum_{i=1}^{N_0} \frac{\partial \vec{V}_i}{\partial t} \cdot \nabla_{\vec{v}_i} N = 0, \quad (2.26)$$

which can be written in convective derivative form

$$\frac{D}{Dt} N(\vec{r}_1, \vec{v}_1, \vec{r}_2, \vec{v}_2, \dots, \vec{r}_{N_0}, \vec{v}_{N_0}, t) = 0. \quad (2.27)$$

The Liouville equation represents the conservation of phase space volume, or the incompressibility of phase space density. Ensemble averaging the phase space density allows the definition of the distribution function for  $N_0$  particle states  $f_{N_0}$ , which gives the probability of finding a system around a particular point in phase space. The distribution function  $f_{N_0}$  is also incompressible

$$\frac{D}{Dt} f_{N_0}(\vec{r}_1, \vec{v}_1, \vec{r}_2, \vec{v}_2, \dots, \vec{r}_{N_0}, \vec{v}_{N_0}, t) = 0. \quad (2.28)$$

Integrating out dimensions gives us distribution functions for any number of particles  $1 \leq k < N_0$

$$f_k(\vec{r}_1, \vec{v}_1, \vec{r}_2, \vec{v}_2, \dots, \vec{r}_k, \vec{v}_k, t) = V^{k-N_0} \int d\vec{r}_{k+1} d\vec{v}_{k+1} \cdots d\vec{r}_{N_0} d\vec{v}_{N_0} f_{N_0}. \quad (2.29)$$

One can integrate equation (2.28) to obtain a hierarchy of equations for  $f_k$ , where each equation for  $f_k$  contains  $f_{k+1}$ . This is the BBGKY hierarchy, and truncating it at  $k = 1$  yields the kinetic equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f + \vec{a} \cdot \nabla_{\vec{v}} f = I[f_2], \quad (2.30)$$

for the single-particle distribution function  $f = f_1$ , where  $\vec{a}$  is the ensemble averaged acceleration of the single particle. The RHS contains the interaction term stemming from the  $f_2$  distribution function. This term is often referred to as the collision operator, or the collision integral.

Another way of deriving equation (2.30) is through using the formalism of Klimontovich, starting from the single particle density function, which contains the 6-dimensional phase space location of each particle

$$N_s(\vec{r}, \vec{v}, t) = \sum_{i=1}^{N_0} \delta[\vec{r} - \vec{R}_i(t)] \delta[\vec{v} - \vec{V}_i(t)], \quad (2.31)$$

and which gives the total number of particles if integrated over the entirety of phase space. Using a similar approach to that used in the derivation of the Liouville equation the Klimontovich equation for  $N_s$  can be obtained

$$\frac{\partial N_s}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} N_s + \vec{a}^m \cdot \nabla_{\vec{v}} N_s = 0, \quad (2.32)$$

where  $\vec{a}^m$  is the microscopic (unaveraged) acceleration of a single particle. In the case of a plasma, this is given by the Lorentz force

$$\vec{a}^m = \frac{q_s}{m_s} \left( \vec{E}^m + \vec{v} \times \vec{B}^m \right), \quad (2.33)$$

where  $q_s$  and  $m_s$  are the particle charge and mass, and the microscopic electric and magnetic fields are given by Maxwell's equations

$$\nabla \cdot \vec{E}^m(\vec{r}, t) = \frac{\rho^m}{\epsilon_0}, \quad (2.34)$$

$$\nabla \cdot \vec{B}^m(\vec{r}, t) = 0, \quad (2.35)$$

$$\nabla \times \vec{E}^m(\vec{r}, t) = -\frac{\partial \vec{B}^m(\vec{r}, t)}{\partial t}, \quad (2.36)$$

$$\nabla \times \vec{B}^m(\vec{r}, t) = \mu_0 \vec{J}^m(\vec{r}, t) + \epsilon_0 \mu_0 \frac{\partial \vec{E}^m(\vec{r}, t)}{\partial t}, \quad (2.37)$$

where the microscopic charge and current densities are given by

$$\rho^m(\vec{r}, t) = \sum_{\text{species}} q_s \int d\vec{v} N_s(\vec{r}, \vec{v}, t), \quad (2.38)$$

$$\vec{J}^m(\vec{r}, t) = \sum_{\text{species}} q_s \int d\vec{v} \vec{v} N_s(\vec{r}, \vec{v}, t). \quad (2.39)$$

In order to obtain the kinetic equation from the Klimontovich equation it is necessary to average over phase space volume, so that

$$N_s = f + \delta N_s, \quad (2.40)$$

$$\vec{E}^m = \vec{E} + \delta \vec{E}^m, \quad (2.41)$$

$$\vec{B}^m = \vec{B} + \delta \vec{B}^m, \quad (2.42)$$

where  $f$  is the average of  $N_s$ , and macroscopic/average fields are given by  $\vec{E}$  and  $\vec{B}$ . The fluctuations average to zero, e.g.  $\langle \delta N_s \rangle = 0$ . Averaging the Klimontovich equation in this manner, gives the kinetic equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f + \frac{q_s}{m_s} \left( \vec{E} + \vec{v} \times \vec{B} \right) \cdot \nabla_{\vec{v}} f = -\frac{q_s}{m_s} \left\langle \left( \delta \vec{E}^m + \vec{v} \times \delta \vec{B}^m \right) \cdot \nabla_{\vec{v}} \delta N_s \right\rangle, \quad (2.43)$$

where the RHS interaction term is now written in terms of the fluctuations of the microscopic fields. Equations (2.30) and (2.43) are identical when applied to the same plasma system. If collisions are ignored, the Vlasov equation is obtained

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f + \frac{q_s}{m_s} \left( \vec{E} + \vec{v} \times \vec{B} \right) \cdot \nabla_{\vec{v}} f = 0, \quad (2.44)$$

used together with averaged Maxwell equations to model collisionless plasmas.

### 2.3.2 Coulomb collisions - the VFP equation

Charged particles colliding in a plasma interact through the Coulomb force. Consider two particles, labeled as the test and field particles, for convenience in treating collisions, with their quantities denoted with subscripts  $T$  and  $F$ , respectively. The equations of motion for these two particles are then

$$m_T \frac{d^2 \vec{r}_T}{dt^2} = \frac{q_T q_F}{4\pi\epsilon_0 |\vec{r}_T - \vec{r}_F|^3} (\vec{r}_T - \vec{r}_F), \quad (2.45)$$

$$m_F \frac{d^2 \vec{r}_F}{dt^2} = \frac{q_T q_F}{4\pi\epsilon_0 |\vec{r}_T - \vec{r}_F|^3} (\vec{r}_F - \vec{r}_T). \quad (2.46)$$

Moving into the centre of mass frame, one can write the equation of motion for the effective particle with reduced mass  $\mu = m_T m_F / (m_T + m_F)$  and position vector  $\vec{r} = \vec{r}_T - \vec{r}_F$

$$\mu \frac{d^2 \vec{r}}{dt^2} = \frac{q_T q_F}{4\pi\epsilon_0 r^3} \vec{r}. \quad (2.47)$$

The deflection angle of the test particle colliding with the field particle can be obtained using standard methods of classical mechanics, deriving expressions for Rutherford scattering. Here the derivation is omitted, and just the general setup defining the quantities described in the collision is shown in Figure 2.9.

The well known result giving the deflection angle in terms of the impact parameter for the case of Rutherford scattering is

$$\tan \frac{\theta}{2} = \frac{q_T q_F}{4\pi\epsilon_0 b \mu v_0^2}, \quad (2.48)$$

where  $v_0$  is the relative velocity at  $r \rightarrow \infty$ . In the case of a plasma, the majority of collisions are small-angle collisions, where  $\theta \ll \pi/2$  [37]. The cumulative effect of such grazing incidence

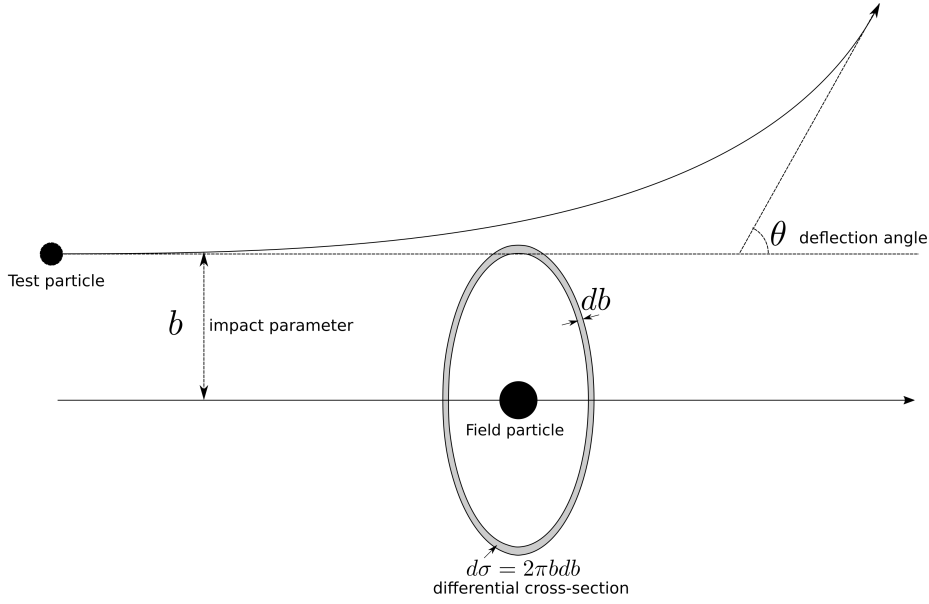


Figure 2.9: Scattering quantities used in the description of Rutherford scattering.

collisions tends to be greater than the effect of much less frequent large-angle collisions. Two length scales govern the relative importance of grazing collisions. The Debye length  $\lambda_D$  gives the largest impact parameter for which collisions are considered, while the impact parameter for which  $\theta = \pi/2$

$$b_{90^\circ} = \frac{q_T q_F}{4\pi\epsilon_0\mu v_0^2}, \quad (2.49)$$

is the lower bound, below which collisions are considered large-angle. These two lengths combine to give the so-called Coulomb logarithm  $\ln \Lambda = \ln(\lambda_D/b_{90^\circ})$  - the greater the logarithm, the better the grazing incidence approximation.

In order to quantify the effect of Coulomb collisions on the distribution function in the grazing incidence approximation, the first step is to consider the conditional probability  $F(\vec{v}, \Delta\vec{v})$  that a particle with velocity  $\vec{v}$  will experience collisions that change its velocity by some  $\Delta\vec{v}$  in a time  $\Delta t$ . The distribution function (that is only being modified by collisions) can be written then as a convolution

$$f(\vec{v}, t) = \int f(\vec{v} - \Delta\vec{v}, t - \Delta t) F(\vec{v} - \Delta\vec{v}, \Delta\vec{v}) d\Delta\vec{v}, \quad (2.50)$$

which basically means that any particle with velocity  $\vec{v}$  at time  $t$  has obtained that velocity via collisions that changed it by  $\Delta\vec{v}$  at time  $t - \Delta t$ . Expanding the integrand in equation (2.50), and using the property of the conditional probability that  $\int F(\vec{v}, \Delta\vec{v}) d\Delta\vec{v} = 1$ , the general Fokker-Planck equation emerges

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \vec{v}} \cdot \left( \left\langle \frac{\Delta\vec{v}}{\Delta t} \right\rangle f \right) + \frac{1}{2} \frac{\partial}{\partial \vec{v}} \frac{\partial}{\partial \vec{v}} : \left( \left\langle \frac{\Delta\vec{v}\Delta\vec{v}}{\Delta t} \right\rangle f \right). \quad (2.51)$$

Here the angled bracket terms

$$\left\langle \frac{\Delta\vec{v}}{\Delta t} \right\rangle = \frac{\int \Delta\vec{v} F(\vec{v}, \Delta\vec{v}) d\Delta\vec{v}}{\Delta t}, \quad (2.52)$$

and

$$\left\langle \frac{\Delta\vec{v}\Delta\vec{v}}{\Delta t} \right\rangle = \frac{\int \Delta\vec{v}\Delta\vec{v} F(\vec{v}, \Delta\vec{v}) d\Delta\vec{v}}{\Delta t}, \quad (2.53)$$

give the classical drag and diffusion coefficients, and represent averages of the velocity change  $\Delta\vec{v}$ . For the case of Rutherford scattering, it can be shown that these coefficients have the following form (see Appendix A for derivation)

$$\left\langle \frac{\Delta\vec{v}}{\Delta t} \right\rangle = \frac{q_T^2 q_F^2 \ln \Lambda}{4\pi\epsilon_0^2 m_T^2} \frac{\partial \mathcal{H}_F}{\partial \vec{v}}, \quad (2.54)$$

$$\left\langle \frac{\Delta\vec{v}\Delta\vec{v}}{\Delta t} \right\rangle = \frac{q_T^2 q_F^2 \ln \Lambda}{4\pi\epsilon_0^2 m_T^2} \frac{\partial^2 \mathcal{G}_F}{\partial \vec{v} \partial \vec{v}}, \quad (2.55)$$

where  $\mathcal{H}_F$  and  $\mathcal{G}_F$  are the so-called Rosenbluth coefficients. These depend on the distribution of the field particles  $f_F$

$$\mathcal{H}_F(\vec{v}) = \frac{m_T}{\mu} \int \frac{f_F(\vec{v}')}{|\vec{v} - \vec{v}'|} d\vec{v}', \quad (2.56)$$

$$\mathcal{G}_F(\vec{v}) = \int f_F(\vec{v}') |\vec{v} - \vec{v}'| d\vec{v}'. \quad (2.57)$$

The Coulomb collision operator in Fokker-Planck form is then given by

$$\frac{\partial f_T}{\partial t} = \frac{q_T^2 q_F^2 \ln \Lambda}{4\pi \epsilon_0^2 m_T^2} \left[ -\frac{\partial}{\partial \vec{v}} \cdot \left( \frac{\partial \mathcal{H}_F}{\partial \vec{v}} f_T \right) + \frac{1}{2} \frac{\partial}{\partial \vec{v}} \frac{\partial}{\partial \vec{v}} : \left( \frac{\partial^2 \mathcal{G}_F}{\partial \vec{v} \partial \vec{v}} f_T \right) \right], \quad (2.58)$$

with the subscripts  $F$  and  $T$  now denoting colliding species in a plasma. When this collision integral is taken as the RHS of equation (2.43) the resulting equation is referred to as the Vlasov-Fokker-Planck (VFP) equation - a widely used tool in the kinetic modeling of collisional plasmas.

### 2.3.3 The Boltzmann collision integral

In the derivation of the Fokker-Planck collision operator, the Rutherford scattering cross-section was used, implying a Coulomb interaction potential. However, what is to be done when particles are interacting with some other potential, specifically a “hard” potential - more akin to billiard balls? This situation arises when a charged particle scatters off an uncharged particle; the interaction is much more localised, and the small-angle scattering assumption breaks down. In this case the Boltzmann collision integral must be utilised. A detailed way of deriving this integral exists, based on the BBGKY hierarchy and hard sphere collisions [53]. However, here an intuitive description of the integral is described, with a simple derivation in Appendix A.

Consider the general case of elastic binary collisions (this can be generalised for inelastic collisions as well). Two particles in the lab frame have initial velocities  $\vec{v}_1$  and  $\vec{v}_2$ , and after the collision their velocities are  $\vec{v}_1'$  and  $\vec{v}_2'$ . Looking at the collision in the centre of mass frame, the relative velocity is given by  $v_{rel}$ . The differential cross section  $d\sigma(v_{rel}, \Omega)$  defines the probability that the relative velocity vector after the collision  $\vec{v}_{rel}'$  will be scattered into the solid angle range  $d\Omega$  around  $\Omega$ . If the distribution to which these particles belong are labeled  $f_1$  and  $f_2$ , the Boltzmann collision integral for  $f_1$  collision integral can be written as

$$\left( \frac{\partial f_1(\vec{r}, \vec{v}_1, t)}{\partial t} \right)_{coll} = \int d\vec{v}_2 \int v_{rel} d\sigma(v_{rel}, \Omega) [f_1(\vec{v}_1') f_2(\vec{v}_2') - f_1(\vec{v}_1) f_2(\vec{v}_2)]. \quad (2.59)$$

In order to understand the Boltzmann collision integral, it is informative to deconstruct it. Firstly, note the assumption that the collisions are localised at some  $\vec{r}$ . The collision integral

gives the change in the number of particles in a phase space volume  $d\vec{r}d\vec{v}_1$  due to collisions. The RHS contains two terms inside the integrand. These are referred to as the gain/absorption and loss/emission terms. The first term, the absorption term, gives all of the particles initially outside of  $d\vec{r}d\vec{v}_1$  that are moved into that volume after collisions. Conversely, the second term, the emission term, counts up the particles that leave  $d\vec{r}d\vec{v}_1$  due to collisions. Note that the concept of pre- and post-collision velocities is different for the two terms. As defined above,  $\vec{v}'_1$  and  $\vec{v}'_2$  are post-collision velocities for the emission term, but pre-collision velocities for the absorption term. When collisions are elastic these can be freely interchanged (see Appendix A), while inelastic collisions require being a little more specific in defining the velocities.

The Boltzmann collision integral is notoriously difficult to treat both numerically and analytically. In Chapter 3 an approach based on the Legendre polynomial expansion of the distribution function is presented, as used in the investigation.

### 2.3.4 Moments of the distribution function - fluid equations

In many cases, even the already simplified approach of the single particle distribution function contains too much information. Sometimes, that information is neither obtainable nor needed, and the fluid approach is taken. In this section the basics of obtaining the fluid equations are covered [52]. The first step here is to define what taking a moment of the distribution function means. For any (scalar, vector, or more generally tensor) function of velocity  $\varphi(\vec{v})$ , its velocity average is

$$\langle \varphi(\vec{v}) \rangle = \frac{\int \varphi f d\vec{v}}{\int f d\vec{v}} = \frac{1}{n} \int \varphi f d\vec{v}, \quad (2.60)$$

where  $n(\vec{r}) = \int f d\vec{v}$  is the density of particles. Taking the moment of the kinetic equation (2.30) amounts to multiplying it by  $\varphi(\vec{v})$  and integrating over velocity space, yielding

$$\int \varphi(\vec{v}) \frac{\partial f}{\partial t} d\vec{v} + \nabla_{\vec{r}} \cdot \int f \varphi(\vec{v}) \vec{v} d\vec{v} + \int \varphi(\vec{v}) \vec{a} \cdot \nabla_{\vec{v}} f d\vec{v} = \int \varphi(\vec{v}) \left( \frac{\partial f}{\partial t} \right)_{coll} d\vec{v}, \quad (2.61)$$

where the above definition of a velocity space average is used, as well as the assumption that  $f$  vanishes for  $v \rightarrow \infty$  (used in partial integration in third term) to rewrite the general moment equation as

$$\frac{\partial(n \langle \varphi(\vec{v}) \rangle)}{\partial t} + \nabla_{\vec{r}} \cdot (n \langle \varphi(\vec{v}) \vec{v} \rangle) - n \langle \vec{a} \cdot \nabla_{\vec{v}} \varphi(\vec{v}) \rangle = n \left\langle \varphi(\vec{v}) \left( \frac{\partial f}{\partial t} \right)_{coll} \right\rangle. \quad (2.62)$$

The standard moment-taking procedure begins by taking  $\varphi = 1$ . This yields the continuity equation

$$\frac{\partial n}{\partial t} + \nabla_{\vec{r}} \cdot (n \vec{u}) = n \left\langle \left( \frac{\partial f}{\partial t} \right)_{coll} \right\rangle, \quad (2.63)$$

where the fluid velocity is defined as  $\vec{u} = \langle \vec{v} \rangle$ . The term on the RHS is the source of particles due to collisions. For simplicity all collision operator moments are dropped in this treatment (see Appendix B for a detailed derivation of fluid equations in the SOL-KiT model, where this is retained). Thus, the simplest form of the continuity equation is

$$\frac{\partial n}{\partial t} + \nabla_{\vec{r}} \cdot (n \vec{u}) = 0. \quad (2.64)$$

It is evident that the continuity equation contains  $u$ , which comes from the next moment, and so it must somehow be obtained. For the next moment equation, setting  $\varphi = m\vec{v}$  gives an equation involving  $u$ , the momentum equation

$$\frac{\partial(nm\vec{u})}{\partial t} + \nabla_{\vec{r}} \cdot (nm \langle \vec{v}\vec{v} \rangle) - nm \langle \vec{a} \rangle = 0. \quad (2.65)$$

The velocity vector is traditionally decomposed as  $\vec{v} = \vec{u} + \vec{w}$ , where  $\vec{w}$  is the random component of the velocity, for which  $\langle \vec{w} \rangle = 0$ , so that

$$\langle \vec{v}\vec{v} \rangle = \vec{u}\vec{u} + \langle \vec{w}\vec{w} \rangle. \quad (2.66)$$

The term  $\mathbf{P} = nm \langle \vec{w}\vec{w} \rangle$  is the so-called pressure tensor, yet another higher moment. For the acceleration the Lorentz force is used (taking particles with charge  $Ze$ ), as in the derivation of

the Vlasov equation. This gives

$$\frac{\partial(nm\vec{u})}{\partial t} + \nabla_{\vec{r}} \cdot (nm\vec{u}\vec{u}) + \nabla_{\vec{r}} \cdot \mathbf{P} - nZe \left( \vec{E} + \vec{u} \times \vec{B} \right) = 0, \quad (2.67)$$

which can be simplified using the continuity equation to obtain the momentum equation

$$nm \left[ \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla_{\vec{r}} \vec{u} \right] + \nabla_{\vec{r}} \cdot \mathbf{P} - nZe \left( \vec{E} + \vec{u} \times \vec{B} \right) = 0. \quad (2.68)$$

The pressure tensor is usually decomposed into a scalar pressure and a viscosity tensor  $\mathbf{P} = p\mathbf{I} + \mathbf{\Pi}$ , where  $\mathbf{I}$  is the identity matrix, and the scalar pressure is expressed in terms of density and temperature  $p = nkT = nm \langle \vec{w}\vec{w} \rangle / 3$ . Thus another equation would be needed for the viscosity tensor and temperature. The temperature equation is usually obtained by setting  $\varphi = mw^2/2$  or  $\varphi = mv^2/2$ , and performing the moment-taking procedure again. Utilizing previous moment equations to simplify, the collisionless temperature equation is obtained

$$\frac{3}{2}nk \left[ \frac{\partial T}{\partial t} + \vec{u} \cdot \nabla_{\vec{r}} T \right] + nkT \nabla_{\vec{r}} \cdot \vec{u} + \nabla_{\vec{r}} \cdot \vec{q} = 0, \quad (2.69)$$

where the second term represents  $p dV$  heating/cooling, and the third term is the divergence of the conductive heat flux, defined as  $\vec{q} = nm \langle w^2 \vec{w} \rangle / 2$ . As previously established, the next moment shows up. For the fluid approach to be of any use, a closure must be defined, so that no higher and higher moment equations are necessary. This can be accomplished either by taking a simple approximation, such as an isothermal plasma with no viscosity, or by using kinetic theory to calculate the higher moments directly. In the detailed derivation in Appendix B, the classical closure due to Braginskii [18] is used. Furthermore, it is necessary to note that the simplified equations presented here are only for one of the species (see appendix and Chapter 3 for the two-fluid equations).

## 2.4 Atomic and molecular processes relevant in the Scrape-Off Layer

As was noted in the review of SOL regimes, neutral particles and their interaction with the plasma can define the system dynamics. Recycling provides a steady supply of neutral particles[54, 35], which then act as a source of plasma through ionisation. Volume recombination becomes increasingly important as the target temperature drops, providing another source of neutral particles. Experimentally, neutral particles can be introduced using approaches such as gas puffing[28], and the interaction of the plasma with the neutrals can provide important diagnostic data through spectroscopy[30]. Here the most important hydrogenic processes will be introduced.

As the focus of the presented research is primarily on the electron dynamics, important electron-neutral collision processes are presented first. The plasmas treated are hydrogenic, so the symbol  $H$  in the following reactions can stand for either hydrogen or deuterium, and the term proton will be used both for  $H^+$  and deuterons  $D^+$ . All collisional processes are characterised by a differential cross section  $d\sigma$ , which is usually integrated over all angles to give the total (or integrated) cross section  $\sigma_{TOT}$ . Finally, one can average the cross section over all velocities of the interacting particles to obtain a reaction rate, which gives the number of reactions per unit time in a unit volume. By using these quantities macroscopic effects of atomic processes can be modeled.

The first process considered is electron impact excitation



where  $n' > n$ . Here,  $n$  can be a shorthand for more complicated atomic states, i.e.  $(n, l)$ , but that is usually not needed[55], and just the principal quantum number  $n$  can be used. The (total) excitation cross-section (for  $1 \longrightarrow n$  transition) as a function of the impacting electron energy is shown in Figure 2.10. As can be seen from the figure, excitation is a process with a defined reaction threshold. The electron energy must be greater than the transition energy between the two atomic states  $n$  and  $n'$ .

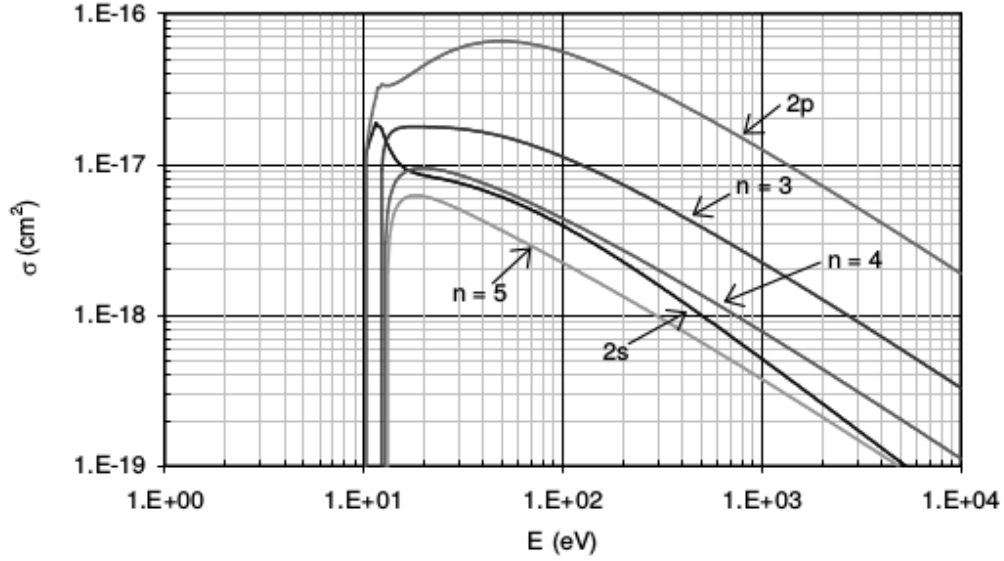
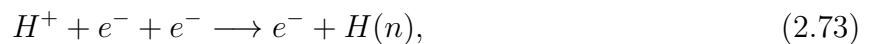


Figure 2.10: Electron impact excitation cross-sections for transitions from ground state. Taken from [55].

Electron impact ionisation acts as a source of plasma in the SOL. While the total number of each reactant (not counting internal states) is conserved in excitation, ionisation does not conserve particle number, as a secondary electron is produced



Even though the numbers of ions and atoms do change, the total number of heavy particles (ions + atoms) is conserved in ionisation reactions. Similarly to excitation, ionisation has a reaction threshold, below which the cross-section vanishes. The inverse of the two processes presented must also be considered. These would be electron impact deexcitation and three-body recombination



whose cross-sections can be obtained using the detailed balance principle (see Chapter 3). While the inverse processes above are important, the main deexcitation and recombination channel is

radiative

$$H(n') \longrightarrow H(n) + h\nu, \quad (2.74)$$

$$H^+ + e^- \longrightarrow H(n) + h\nu, \quad (2.75)$$

where  $h\nu$  is the photon carrying away the reaction energy. One can then ask the question "Should we include photon absorption in the form of radiative excitation and ionisation?". While this is possible [56], the SOL is usually treated as optically thin, so any photons are assumed to escape the plasma without interacting, which is why only photon-emitting processes are discussed.

Proton impact excitation and ionisation also occur, and can potentially be important due to non-negligible ion temperatures. These two reactions,

$$H^+ + H(n) \longrightarrow H^+ + H(n'), \quad (2.76)$$

$$H^+ + H(n) \longrightarrow H^+ + H^+ + e^-, \quad (2.77)$$

are, in the same vein as the electron impact reactions, subject to an energy threshold. However, there is a proton impact process which does not have an energy threshold. This is charge-exchange

$$H^+ + H(n) \longrightarrow H(n) + H^+, \quad (2.78)$$

where the impacting proton transfers its charge to the neutral, but largely retains its momentum. The scaled cross-sections for this process are given in Figure 2.11.

Macroscopically, charge exchange is experienced as friction by the ions, while the produced fast neutrals can emit Doppler-shifted radiation, which can in turn be picked up and used by the spectral diagnostics[57].

While other more exotic atomic processes exist, such as  $H^-$  ion formation [55], molecules are the culprits behind the overwhelming complexity of low temperature hydrogenic plasmas.

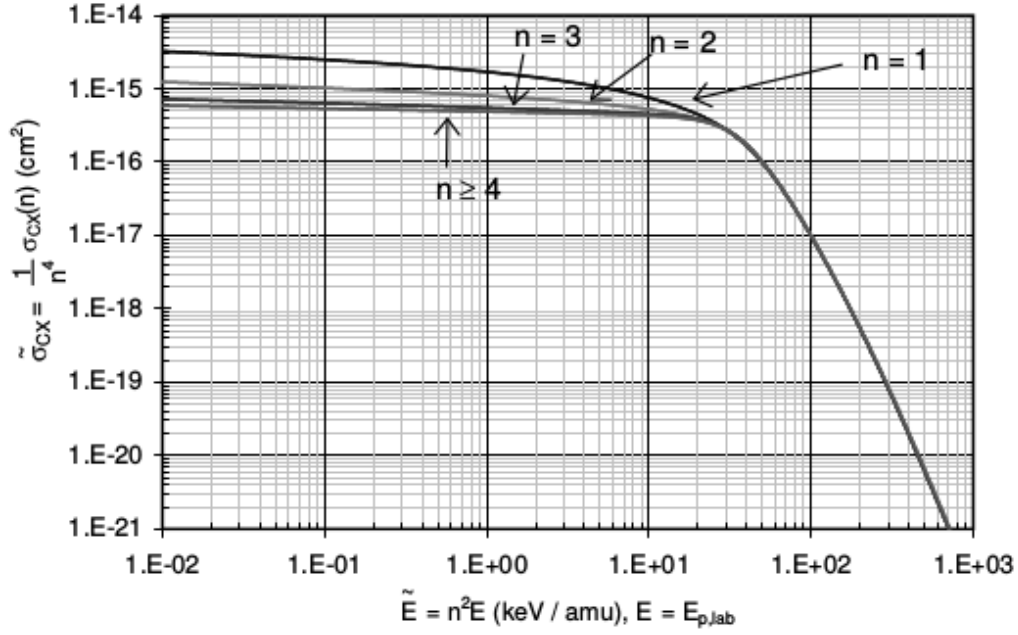
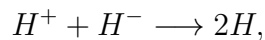
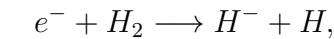


Figure 2.11: Charge exchange cross-section, scaled. Impacting proton energy given in lab frame. Taken from [55].

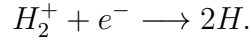
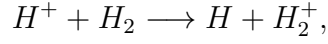
As molecules have a greater diversity of internal states, the excitation and ionisation processes become much more complicated. However, there are further complications in dealing with molecules, the first of which is the addition of association and dissociation reactions. An example would be electron attachment dissociation, which also produces  $H^-$  ions



where the actual reaction can proceed via multiple intermediate channels. The atomic hydrogen in the SOL is produced in similar reactions, as the recycled particles leave the surface in molecular form. Those molecules then dissociate, and, due to the Franck-Condon principle[58, 59], the resulting atoms can have very high energies [12]. Further complications arise when charge exchange is included, as well as reaction chains. An example of a reaction chain potentially important in the SOL is the following Molecule-Activated Recombination (MAR) chain [60]



where electron attachment dissociation is followed by mutual neutralisation of  $H^-$  and  $H^+$ . Another example of MAR is molecular charge-exchange followed by  $H_2^+$  dissociative recombination



Either of the above reaction chains effectively reduces the number of electron-ion pairs, hence acting like recombination. As such, molecules bring an important qualitative change in the plasma behaviour, as well as the quantitative changes in plasma-neutral friction and radiative power loss. It is therefore natural to assume they would play a key role in detachment. However, the study presented in the later chapters of this text is limited to atomic effects as a first step to incorporating neutral physics.

## 2.5 Edge-Localised Modes and other transients

In H-mode, the high confinement mode in a tokamak, a particular type of MHD instability is observed, coined the Edge-Localised Mode (ELM)[12]. While the exact cause of the instability is not yet fully understood, one of the explanations offered in the literature is that of the coupled peeling-ballooning mode[61, 62]. The instability is driven by a combination of current (peeling) and pressure (ballooning) in the pedestal region. The simplified picture of a pedestal is a steep pressure drop just before the separatrix in H-mode, associated with a reduction of transport[63]. A standard signature of an ELM is a sharp increase in the observed  $D_\alpha$  line radiation.

Reported ELMs come in three flavours[12]:

- Type I: These are the giant ELMs that can eject up to 10% of the energy stored in the core in each burst. They have relatively low frequencies, 1 – 100 Hz, that increase as the input power is increased. Of all three types, these are considered to be by far the most dangerous to the PFCs.
- Type II: Uncommon low power ELMs observed in highly shaped plasmas. The energy loss is much smaller than 1% of the contained energy.

- Type III: High frequency ELMs observed just above the L - H transition heating power threshold. Energy loss is typically on the order of 1%, and frequencies are high, 0.1 – 1 kHz. Unlike Type I ELMs, the frequency drops with increasing heating power.

A simplified diagram showing the stability region for peeling-ballooning modes in the pedestal is given in Figure 2.12. The stability region is plotted in pedestal current-pressure space, and the three types of ELMs discussed above are marked on the edge of the stable region.

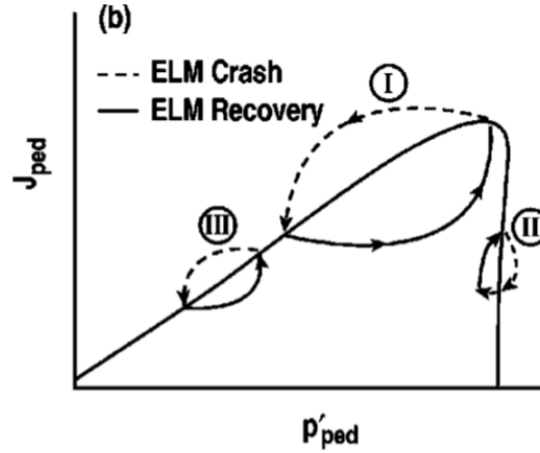


Figure 2.12: A simplified ELM stability diagram. Different ELM types are marked on the edge of the stable region. Taken from [62].

ELMs are a source of both particles and energy, with Type I ELMs releasing up to 15% of the core particle content into the SOL. In the discussion on previous kinetic modelling that follows this section, both Type I and Type III ELM simulations are discussed. It is worth noting here that Type III ELMs have kinetically been simulated as just an energy perturbation[2]. This is similar to the perturbation simulations performed in the study presented in this thesis. However, the author has consciously chosen not to use the term “ELM” when describing these purely conductive transients, as no upstream particle sources were used.

As mentioned briefly in the previous chapter, transients other than ELMs can be present in the SOL. These can be diagnostic gas puffs[28], heating pulses, as well as L-mode filaments/blobs[13]. While a wide accounting of all transients in the SOL is well beyond the scope of this text, it is worth noting that not just ELMs could be an interesting topic. For example, when modelling cross-field transport of filaments in L-mode using a statistical framework[17], one of the input parameters is the parallel energy decay time, which is governed by parallel transport. As such,

kinetic effects in model parallel transients could be used to inform higher-dimensional models of said transients. Similarly, if there are kinetic effects in the atomic physics, these could potentially be used to inform spectroscopic models.

## 2.6 Overview of plasma non-locality in the SOL

In order to further motivate the study presented in this work, as well as provide background for the interpretation of results, an overview of non-locality research in the SOL will be presented. Ad hoc and empirical modelling will be reviewed first, while the various kinetic approaches to SOL modelling will follow. This review is limited to electron phenomena so as to remain relevant to results presented in later chapters. However, in the interest of completeness, non-electron kinetic effects will be mentioned as they appear in the presented studies.

### 2.6.1 Basic concepts and flux limiters

As was noted in Chapter 1, in order to use a classical result such as equation (2.10), high collisionality with respect to the system scale is required. In the SOL the parallel scale is the connection length  $L$  (see Section 1.3 of this chapter). However, this is not the most relevant length scale when determining the importance of kinetic effects [19]. The parallel temperature gradient scale length  $L_{\nabla T} = (\nabla_{\parallel} T/T)^{-1}$  is much more appropriate, and can be computed for each species in the plasma. If  $\lambda_{ss}$  is the self-collision mean free path of species  $s$  the Knudsen number can be defined as  $K_{T_s} = \lambda_{ss}/L_{\nabla T_s}$  to act as a measure of non-locality. This is also compatible with the short mean free path requirement  $K_{T_s} \ll 1$  of the Chapman-Enskog expansion [64] in thermodynamic equilibrium. The standard collisionality parameter used in the SOL  $\nu^* = L/\lambda_u$  is also recovered when  $\nabla T \rightarrow 0$  so that  $L_{\nabla T} \rightarrow L$ , when  $K_{T_s} \approx 1/\nu^*$ .

The total parallel heat flux of species  $s$  is given by

$$q_s^{TOT} = \frac{m_s}{2} \int d\vec{v} v^2 v_{\parallel} f_s = \left( \frac{5}{2} k T_s + \frac{1}{2} m_s u_s^2 \right) n_s u_s + q_s, \quad (2.80)$$

where  $q_s$  is the conductive heat flux given by (2.10). As collisionality is reduced, a long mean free path regime ensues, assuming that the plasma is still quasi-Maxwellian gives the free streaming

one-sided heat and particle fluxes [19]

$$q_s^{FS} = \frac{m_s}{2} \int_0^\infty dv_{||} \int_{-\infty}^\infty dv_{\perp} v^2 v_{||} f_s = 2kT_s \Gamma_s^{FS}, \quad (2.81)$$

$$\Gamma_s^{FS} = \int_0^\infty dv_{||} \int_{-\infty}^\infty dv_{\perp} v_{||} f_s = \frac{1}{4}(8\pi)^{1/2} n_s v_{ts}, \quad (2.82)$$

where  $v_{ts} = (kT_s/m_s)^{1/2}$ . If the plasma is devoid of source and field variations, the heat flux is limited by the free streaming flux since  $\nabla T_s \rightarrow 0$  and the classical conductive heat flux vanishes. However, this is not the case in the SOL, and a temperature gradient can exist even when the mean free path tends to infinity. This causes the Spitzer-Härm heat flow [46] to grow without bounds, and can no longer be used unmodified. Standard practice in this case is to limit the conductive heat flux to some fraction  $\alpha_s$  of the free streaming value  $q_s^{FL} = \alpha_s kT_s n_s v_{ts}$  by writing

$$q_s = \frac{q_s^{SH}}{1 + |q_s^{SH}/q_s^{FL}|}, \quad (2.83)$$

where  $q_s^{SH}$  is given by (2.10).  $\alpha_s$  is often referred to as the flux limiter, and its value seems to heavily depend on the parameters of the SOL, with electron values reported in the literature [19] varying from less than 0.03 to values as high as 0.8. This value can also vary in time, and values greater than 1 have been reported, pointing to the effect of flux enhancement. Further drawbacks of using a flux limiter will be explored both in this section, as well as in the result chapters. It is worth noting, however, that flux limiters have been used successfully for interpretative simulations of both L- and H-mode SOL profiles [65, 66].

### 2.6.2 Overview of electron kinetic modelling

In this section a review of a number of electron modelling results from the literature will be presented. The selection was made in order to illustrate the development of the field as well as showcase some of the results used to motivate the present study. The section is structured as follows. After introducing an important concept for non-local transport the focus will be shifted to individual approaches that best illustrate the state of the field of electron non-local transport

in the Scrape-Off Layer.

### Heat-carrying electrons

Discrepancies between 2D fluid code simulations and experiments have been investigated by Chankin and Coster [1]. One of the proposed potential causes of the observed discrepancies is “...non-local kinetic effects in the parallel plasma transport (poorly accounted for in the [fluid] codes).” An important concept in understanding non-local transport is that of the heat-carrying electrons (HCE). Heat carrying electrons are those electrons in the electron distribution function  $f_e$  that contribute the most to the integral in equation (2.80), i.e. those for which  $v^2 v_{||} f_e$  is at its maximum. Since the mean free path for Coulomb collisions  $\lambda \propto v^4$ , even if thermal electrons with velocities of order  $v_{th} = \sqrt{kT_e/m_e}$  have relatively low Knudsen numbers, a sufficiently fast electron population would be much less collisional than the thermal bulk of the distribution. Thus, if the HCE have a large velocity they can be marginally collisionless. This is exactly the result accepted in the literature, with HCE velocities reported in the range  $v_{HCE}/v_{th} = 3.45 - 3.75$  [67, 68], giving  $\lambda_{HCE}/\lambda_{th} > 141$ . However, a more conservative estimate  $\lambda_{HCE}/\lambda_{th} \approx 20 - 50$  was given by Chankin [68] by taking into account the parallel-perpendicular anisotropy of the distribution function. Nonetheless, even with this increase in collisionality the HCE will be collisionless for plasma conditions in the SOL.

### Pre-2000 SOL kinetic modelling

During the 90s, a number of codes were developed and utilised in the study of electron parallel transport. Examples include both PIC [69] and finite difference Vlasov-Fokker-Planck codes [2, 70]. Various degrees of sophistication in the treatment of the plasma and neutral particles were present.

The 1D Particle-in-Cell (PIC) code DIPSI was used by Procassini et al. [69, 71] to simulate a divertor in the high recycling regime. In order to overcome the computing limitations at that time a reduced ion-electron mass ratio  $m_i/m_e = 200$  was used, as well as simulating a short system ( $L = 2.1\text{cm}$ ). Non-local effects are observed in both the limiting of the heat flux, as well as the modification of the sheath heat transmission factor. Both were shown to be a function of

the recycling intensity. The neutral distribution in the PIC code was given by an exponential function, dropping off away from the divertor target.

Another approach to modelling a recycling divertor was taken by Abou-Assaleh et al.[72, 70] by coupling the Vlasov-Fokker-Planck code FPI[73] to a 1D two-fluid code. The FPI code uses a Legendre decomposition of the electron distribution function, similarly to the code developed during the study presented in this work (see Chapter 3). Interactions with neutrals are included on a kinetic level, while the results were compared with those performed using just the fluid code. Significant discrepancy was observed even when a flux limiter was utilised in the fluid code.

The most sophisticated code developed during this time period, and arguably one of the most detailed 1D VFP codes used in the simulation of SOL transport, is the ALLA code developed by Batishchev et al.[2, 74, 75, 76, 77] It contains kinetic equations for both the electrons and the ions, as well as a simplified kinetic equations for the neutrals. Rosenbluth coefficients are computed for the Coulomb collisions, while inelastic collisions are treated self-consistently using the Boltzmann collision integral. Charge exchange collisions are included using

$$C_{CX} = \int \sigma_{CX} |\vec{v} - \vec{u}| [f_N(\vec{v}) f_i(\vec{u}) - f_i(\vec{v}) f_N(\vec{u})] d\vec{u}, \quad (2.84)$$

where  $f_N$  and  $f_i$  are the neutral and ion distribution functions, respectively. Neutral-neutral collisions are approximated using the BGK[78] collision operator

$$C_{NN} = \nu_{NN} (f_N^M - f_N), \quad (2.85)$$

where the drifting Maxwellian  $f_N^M$  has the same first three moments as  $f_N$ , and  $\nu_{NN}$  is the neutral-neutral elastic collisions frequency. The electric field is computed using the ambipolar flow constraint, and balances ion and electron pressure and friction. ALLA utilises the logical boundary condition[69], where the sheath at the target is simulated by introducing a cut-off in the electron distribution. The cut-off represents the fact that any electron with enough energy to overcome the sheath potential is lost, and is thus not seen in the backwards-going part of the distribution. The logical boundary condition will be addressed in more depth in Chapters 2 and

3 in the context of the Legendre decomposition of the distribution function.

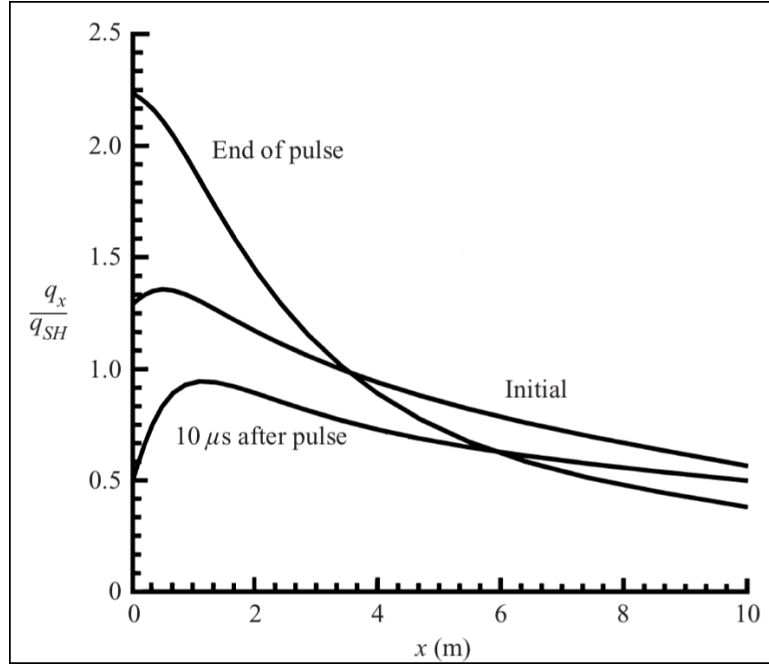


Figure 2.13: The ratio of the calculated heat flux to Spitzer-Härm value during ALLA runs of transients for Alcator C-Mod conditions[2]. Note the strong effect of the heating pulse both during and after the heating period.

ALLA simulations are reported to agree well with multiple experiments and on several machines, including Alcator C-Mod, DIII-D, and Tokamak-de-Varennes (see [2] and references therein). Figure 2.13 shows the evolution of the ratio of the computed electron heat flux to the classical Spitzer-Härm value during a non-stationary regime in Alcator C-Mod conditions. Here the zero on the  $x$ -axis marks the target. A realistic deuterium mass ratio  $m_i/m_e = 3672$  was employed, with line-averaged density  $\langle n_e \rangle = 6 \times 10^{19} \text{m}^{-3}$  and  $L = 10 \text{m}$  connection length. Steady state heating was implemented using a diffusive operator, and the effective heating heat flux was set to  $q_x = 30 \text{MW m}^{-2}$ . Non-stationary regimes were reported for an increase in  $q_x$  by a factor of order 10 during a  $10 \mu\text{s}$  period. From Figure 2.13 it is evident that the transient event (interpreted as a type III Edge-Localised Mode) strongly affects the electron heat conductivity.

Strong kinetic effects are observed in ALLA runs for all species in the simulations, indicating their importance in both steady state and transient situations. However, the work treats a limited number of plasma regimes, and does not offer a comparison to equivalent fluid runs in order to isolate kinetic effects. Some of these points are treated in later research (see below), while the original research presented in this work will attempt to address both points.

**SOL kinetic modelling 2000-present**

PIC codes have been and remain a workhorse in the exploration of the kinetics in the SOL. As mentioned above, early PIC codes used a reduced ion-electron mass ratio to speed up convergence[69], but with the increase in computing power this constraint has been largely lifted, and massively parallelised PIC codes became possible. The main example of such a code is BIT1 [79], which is a 1D PIC code capable of simulating a variety of species and processes, giving it a unique position in SOL research.

BIT1 has been used extensively in simulating present day machine conditions, primarily those at JET [80, 4]. Simulations performed using BIT1 explored both electron and ion kinetic effects, both in equilibrium, as well as during ELMs. ELMs were simulated as both a density and temperature perturbation in the upstream SOL. Limiters and sheath properties (heat transmission coefficient and potential drop) are referred to as kinetic factors (KF) by the authors, and they show that all KF depart strongly from their classical values during ELMs, while the classical values seem to work well for the equilibrium case [80]. Parallel ion heat flow has been explored as a function of collisionality, and BIT1 was used to test the validity of the Bohm criterion for a high-recycling regime [4].

Impurities have been treated kinetically using BIT1, as well. A deuterium plasma in JET relevant conditions was simulated, with the inclusion of  $C^{+m}$  and  $W^{+n}$  ( $m = 0, \dots, 2$ ,  $n = 0, \dots, 11$ ) species [81]. Tungsten ionisation states were observed only up to  $n = 4$ , and it was noted that at the used particle density accuracy was not sufficient to study the tungsten state distribution in the upstream SOL. BIT1 has also been used together with the erosion code ERO to study tungsten deposition [82].

Inelastic collisions with hydrogenic species are also treated consistently in BIT1, including both three-body and radiative recombination [83]. Finally, a number of studies of kinetic effects on probe measurements have been performed using the PIC code [84, 85]. It was found that Langmuir probe measurements overestimate equilibrium temperatures due to the presence of fast particles, while the fast dynamics during ELMs cause the probe measurements to underestimate the target temperatures [85].

The final code to be covered in this section is the newly developed finite difference code

KIPP [86]. It is most closely related to ALLA, discussed above, with the main difference being that KIPP does not treat ions or neutrals, and instead uses preset profiles, maintained through the use of particle and power sources [5]. KIPP is developed with the explicit intention of being coupled with existing SOL fluid codes, and first steps toward this sort of coupling have been performed [87, 88, 89].

Extensive benchmarking was performed with KIPP, ranging from testing the electron-ion temperature equilibration rates [90], to the reproduction of local/classical transport results [91]. As mentioned at the beginning of this section, KIPP was used to examine the anisotropy of the distribution function in the context of heat-carrying electrons [68].

KIPP was used to perform a collisionality scan while exploring different particle and energy source operators [5]. While there was no substantial difference between the profiles obtained using different implementations of sources, non-monotonic behaviour of the electron sheath heat transmission with respect to collisionality was observed, similar to that reported in [80]. It is worth noting that the background profiles were taken with a parabolic flow velocity profile, while electron and ion temperatures were assumed equal.

Profiles based on JET highly radiative H-mode shots obtained using the fluid and Monte Carlo code package EDGE2D-EIRENE were used as a first attempt at coupling KIPP with a fluid code [87]. By taking EDGE2D profiles along field lines at different radial positions (slices), several KIPP runs were performed, utilizing sources to maintain the input fluid profiles, but allowing the electron distribution function to relax to a kinetic equilibrium. This allowed for the calculation of the parallel electron heat flux, as well as the sheath properties, in a kinetic way. While all of the slices had similar upstream collisionality, due to nitrogen radiation (simulated in the fluid codes), the different slices had very different target temperatures, ranging from detached to completely attached. Both flux suppression and enhancement were observed, with the heat flux suppressed throughout most of the SOL, while the enhancement was close to the target. The sheath properties were also affected, but neither deviated too strongly from those assumed by the fluid code. However, the authors note that the explored regimes were limited, and that a number of factors could change the kinetic effects from merely present to more dominant. Firstly, the introduction of a kinetic treatment of ions and of atomic process

rates could affect the solution. An iterative scheme for coupling KIPP to fluid codes has since been developed that incorporates atomic processes in the kinetic model[92, 88, 89], and kinetic effects on ionisation have been found to be negligible in the explored SOL equilibrium scenario.

### Comparative simulation of transients in the SOL

An illustrative cross-code comparison between two kinetic codes and a 1D fluid code [93] was performed by Havlíčková et al. [94]. The two kinetic codes were the PIC code BIT1[79] (discussed above), and a Vlasov (collisionless) code [20]. All three codes were used to simulate the energy fluxes to the target in a weakly collisional case corresponding to a JET ELM, where the connection length was taken to be  $L = 40\text{m}$ . The ELM was modelled as a particle and energy perturbation upstream, with hot particles with a temperature of  $1.5\text{keV}$  being injected at sound speed from a population with density  $5 \times 10^{19}\text{m}^{-3}$  over parallel length of  $\approx 25\text{m}$  and during a time period of  $t = 200\mu\text{s}$ . Figure 2.14 shows the evolution of the energy flux at the target obtained with the three different codes. Three distinct stages are observed in the evolution of the energy flux  $Q$ . Before  $t \approx 10\mu\text{s}$  fast particle transport is observed in the PIC and Vlasov codes, while the fluid code does not see this effect. From  $\approx 10 - 80\mu\text{s}$  conduction dominates, and the fluid code overestimates the value of the conductive flux. Finally, after  $\approx 80\mu\text{s}$ , the bulk of the hot ELM particles begins arriving in the convective phase of the transient. From the dominance of that third phase it can be seen that the reference case examined by the authors was indeed a convective transient. The authors also note that an analytical free-streaming model [26] describes the main features of the target energy flux.

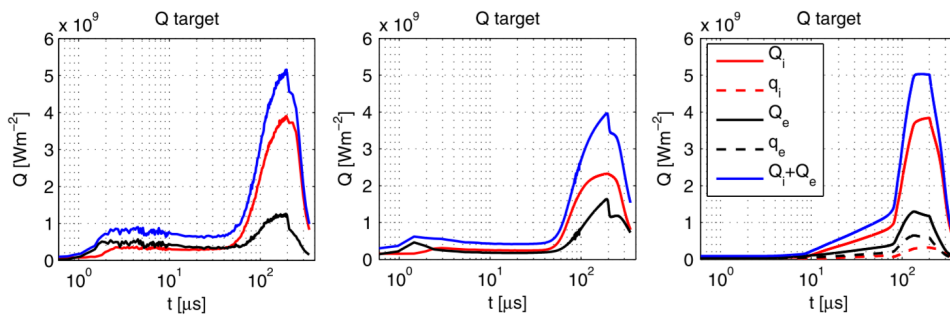


Figure 2.14: Evolution of the energy flux at the target obtained by Havlíčková et al. [94] using (left) BIT1, (centre) a Vlasov code, (right) and the SOLF1D fluid code. Dashed lines in the fluid code results show the conduction contribution to the energy flux.

It is important to note that recycling and plasma-neutral interaction were not treated in this comparison study, and that the collisionality of the reference case was low. No heat flux limiters were employed by the fluid code. Instead, the viscosity was limited, and the energy source was modified in order to match the results of the kinetic codes. More specifically, the kinetic codes assume that the source energy is distributed equally between ions and electrons, whereas the fluid code had to employ a 3:1 split between the energy given to the ions and the electrons. This artificial modification is justified by the fact that the boundary condition in the fluid code assumes no variation in sheath potential, while the kinetic codes calculate its value as it changes during the ELM. It is argued that as the sheath potential increases, the energy flux due to electrons is suppressed, since a smaller number of them have the required energy to overcome the potential.

Havlíčková et al. report that the inclusion of spatially uniform and constant (in time) heat flux limiters reduces the agreement between the kinetic and the fluid codes. They go on to discuss that, while the discrepancy between the different models was small in the case of the reference convective transient, shorter conductive transients would likely increase the difference between the outputs of the kinetic and fluid models. Quoting the authors: “Results show that the validity of the fluid model is disputable if the heat conduction plays the major role in the power deposition at the target”. In Chapters 5 and 6 of this work this particular case of short conductive transients is examined using the code that will be introduced in the following two chapters.

## 2.7 Summary

The area of exhaust physics is rather broad, with topics ranging from the focus of this thesis, parallel transport, to various turbulent and diagnostic phenomena, such as L-mode filaments[13] and gas puffs[28]. In this chapter, the basic concepts necessary for the upcoming discussion have been covered. The SOL has been introduced, with a special focus on the divertor configuration, which enables H-mode and detachment, a beneficial operating regime that protects the plasma facing components through a neutral cloud buffer. Various SOL regimes have been introduced

via the simple Two-Point Model, connecting them with a variation in collisionality.

Tools necessary for the discussion of kinetic methods have also been reviewed, with the kinetic equation, collisions, and the moment-taking procedure of obtaining fluid equations covered. As both Coulomb and electron-neutral collisions are of interest in the present study, both the Fokker-Planck collision integral, as well as the Boltzmann collision integral have been presented, with simple derivations partly relegated to Appendix A.

A very basic review of atomic and molecular processes in the SOL has been given. Electron processes such as impact excitation and ionisation, as well as their inverse processes of deexcitation and recombination are discussed. The most important of ion processes, charge-exchange, has also been included. While outside of the scope of this study, interesting and important molecular effects were also considered.

Finally, a very brief introduction to ELMs is followed by a review of non-locality modelling in the SOL. Concepts such as flux limiters and heat-carrying electrons have been introduced and used in going over the main results from the literature. Previously observed kinetic effects include everything from flux suppression and enhancement, boundary condition modification, as well as ionisation rate effects. However, these were all observed in very machine-specific regimes, and the aim of the study to be presented in the remainder of this thesis is to both expand on the modelling methodology, as well as use the updated methods to contribute to the study of equilibria and transients in parallel electron transport in the SOL. Of special interest is the interaction of transients with detachment, and as such electron-neutral interactions will play an important role in the upcoming discussion.

Before moving on to presenting what has been done, it is worthwhile to step back and consider what has been omitted through the choice of focal point. As the focus of this study is kinetic effects in parallel electron transport, this naturally excludes both cross-field transport, and non-electron kinetics. In excluding cross-field transport, phenomena such as filaments and other turbulent structures, as well as the transport of neutrals in the complex geometry of a realistic SOL have all been ignored. Increasing the dimensionality and including magnetic field geometry would open doors to far more realistic simulations, but would almost certainly require a change in approach as the finite difference method of solving the kinetic equation

presented in this thesis would likely not scale well. As such, the choice to restrict the study to parallel transport is made partly out of necessity. Similarly, adding a kinetic treatment of ions and neutrals would also increase the breadth of the study, and these are tentatively planned extensions of the study.

# Chapter 3

## SOL-KiT model

### 3.1 Overview of the SOL-KiT model

A considerable part of the PhD project presented in this text has been dedicated to the development and testing of the new electron kinetic transport code SOL-KiT (**S**crape-**O**ff **L**ayer **K**inetic **T**ransport). The aim was to develop a self-consistent modular tool for the exploration of electron kinetic effects in the SOL, which would be capable of providing systematic insight into the fundamental departures from the classical fluid results. In this section a basic overview of the model is given, while the rest of the sections in this chapter will focus on the individual aspects of the model. In the next chapter the basis of the model presented here will be used to develop the practical implementation in SOL-KiT.

While the code is capable of handling both fixed and periodic boundary conditions, since the most involved cases utilise the Scrape-Off Layer domain, it is described here. The domain is 1D, and is assumed to be along a straightened field line (much in the same vein as the Two-Point Model setup in the previous chapter). The field line is taken as the  $x$ -axis, around which the domain is symmetric. The point  $x = 0$  is taken to be at the symmetry plane, representing the “upstream” of the SOL. A sketch of the simplified SOL domain is given in Figure 3.1.

When fully utilised, the SOL simulation scenario includes sources in the upstream, a sink at the divertor target, where plasma recycling occurs, and plasma flows interacting inelastically with the neutral cloud being formed due to recycling.

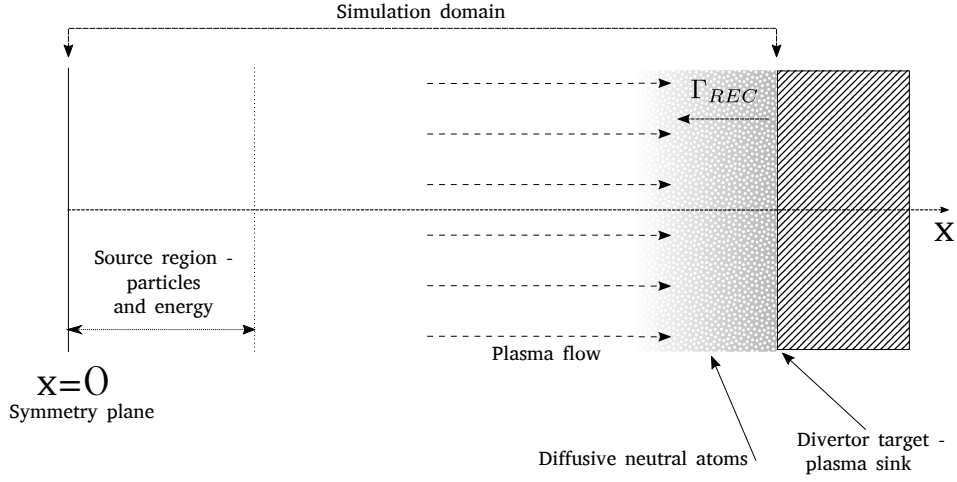


Figure 3.1: The SOL simulation domain (not to scale): the  $x$ -axis is the principle axis of the system, with  $x = 0$  being the upstream symmetry plane; the right boundary of the system is at the divertor target, which acts as a sink for the plasma, as well as a source of neutrals via the recycling flux  $\Gamma_{REC}$

As was noted in the literature review in section 2.6, a number of numerical modeling tools have been developed for the study of SOL kinetics. While extensive kinetic models[2, 79] exist, and some of them have been compared with fluid codes on a limited number of problems [94], there has been no attempt to systematically explore the fundamental aspects of kinetic transport in the SOL. As has already been stated, SOL-KiT was developed as a platform for such fundamental investigations. The first step towards a systematic comparison is ensuring a one-to-one correspondence between a fluid and kinetic model for the electron transport. For this reason, SOL-KiT includes two modes for the simulation of electrons:

- The kinetic mode, where the Vlasov-Fokker-Planck-Boltzmann equation for the electrons is solved

$$\frac{\partial f(x, \vec{v}, t)}{\partial t} + v_x \frac{\partial f(x, \vec{v}, t)}{\partial x} - \frac{e}{m_e} E \frac{\partial f(x, \vec{v}, t)}{\partial v_x} = C[f, \dots], \quad (3.1)$$

where  $E$  is the electric field (assuming azimuthal symmetry and straightening out the magnetic field magnetic effects are ignored). The RHS contains all of the collision and source operators. The kinetic equation is solved by utilizing a decomposition in Legendre polynomials, covered in section 3.4, where all of the individual operators are presented.

- The fluid mode, where the continuity, parallel momentum, and temperature equations are

solved for the electrons.

Along with the equations for the electrons, ion continuity and momentum equations can be solved, and the electric field  $E$  is calculated using Ampère-Maxwell’s law. The general equations appearing in any mode, along with the electron fluid equations, will be the topic of section 3.2.

Discussed separately, the atomic processes and the equations governing the evolution of atomic states will be presented in section 3.3. Finally, a novel method of treating the logical boundary condition in the Legendre formalism will be presented in 3.5.

As each aspect of the model is introduced, the motivation behind its inclusion and chosen treatment will be elaborated. Any derivation pertinent to the main discussion will be included as well, while more cumbersome and purely technical aspects will be relegated to appendices.

## 3.2 Fluid and general mode equations

As noted in the previous section, the electrons in SOL-KiT can be treated as a fluid. This involves the solving of three equations for the moments of the kinetic equation. Care has been taken in deriving the equations to be consistent with the kinetic model, and this derivation can be found in Appendix B. In this section the electron equations will be presented and described, followed by the equations for the ion quantities and the electric field.

The electron continuity equation determines the evolution of the electron density  $n_e$ , and with sources included is given by

$$\frac{\partial n_e}{\partial t} + \frac{\partial(n_e u_e)}{\partial x} = S, \quad (3.2)$$

where  $S = S_{ion} + S_{rec}$  is the particle source including ionisation and recombination (the exact forms are covered in the section 3.4 as well as in Appendix B). The source term can also be externally set, and will be covered in the section on the kinetic mode. As the continuity equation requires having the electron flow velocity  $u_e$ , the parallel momentum equation must be solved. With all of the physics included in the SOL-KiT model, this equation is given by

$$\frac{\partial u_e}{\partial t} = -u_e \frac{\partial u_e}{\partial x} - \frac{e}{m_e} E + \frac{R_{ei} + R_{en}}{m_e n_e} - \frac{S}{n_e} u_e - \frac{1}{m_e n_e} \frac{\partial(n_e k T_e)}{\partial x}, \quad (3.3)$$

where two friction terms  $R_{ei}$  and  $R_{en}$  need to be defined. The first, electron-ion friction, is given by the classical Braginskii[18, 47] friction  $R_{ei} = R_T + R_u$  where

$$R_u = -\frac{m_e n_e}{\tau_e} 0.51(u_e - u_i), \quad (3.4)$$

$$R_T = -0.71 n_e \frac{\partial(k T_e)}{\partial x}. \quad (3.5)$$

In the above expressions  $\tau_e$  is the Braginskii collision time [18, 47]

$$\tau_e = 3.44 \times 10^{11} \frac{T_e[\text{eV}]^{3/2}}{n_e[\text{m}^{-3}] \ln \Lambda} \text{s}. \quad (3.6)$$

The friction felt by the electrons from collisions with neutrals  $R_{en}$  includes all the possible electron-neutral interactions, and will be discussed along with the sources in section 3.4. The last term in the momentum equation is the electron pressure gradient force. To calculate the temperature necessary for this term and the frictional terms, it is necessary to solve the third and final electron fluid equation in the model, the temperature equation

$$\frac{\partial k T_e}{\partial t} = -u_e \frac{\partial k T_e}{\partial x} + \frac{2}{3} \left[ \frac{Q}{n_e} - k T_e \frac{\partial u_e}{\partial x} - \frac{1}{n_e} \frac{\partial q_e}{\partial x} - \frac{S}{n_e} \left( \frac{3}{2} k T_e - \frac{m_e u_e^2}{2} \right) - \frac{u_e (R_{ei} + R_{en})}{m_e n_e} \right]. \quad (3.7)$$

Equation 3.7 contains a variety of terms on the RHS (see Appendix B and section 3.4), including two source terms, one from the particle source as seen in equation 3.2, and another due to a combination of external heating and the collisions with neutrals  $Q = Q_{ext} + Q_{en}$ . The second and last terms in the parentheses of equation 3.7 are the pdV heating and frictional energy exchange terms, respectively. Finally, the conductive heat flux  $q_e$  would require another equation to specify, but SOL-KiT utilises the closure by Braginskii[18]  $q_e = q_T + q_u$  where

$$q_T = -\kappa_e \frac{\partial(kT_e)}{\partial x}, \quad (3.8)$$

$$q_u = 0.71n_e kT_e (u_e - u_i). \quad (3.9)$$

The heat conductivity  $\kappa_e$  is given by the updated Spitzer-Härm result[46, 95]

$$\kappa_e = 3.2 \frac{n_e kT_e \tau_e}{m_e}, \quad (3.10)$$

or can be specified by using another approximation (for example the Lorentz approximation result by Epperlein[96]).

In both the fluid and kinetic electron modes the ions are treated as a fluid, analogously to the above treatment of electrons, with a few differences. Firstly, the ion continuity equation can be solved, or quasi-neutrality can be enforced artificially by setting  $Zn_i = n_e$ . Secondly, there is no ion temperature equation in the current version of the model. Instead, ion temperature is set to either zero, or to the electron temperature. The ion equations are then

$$\frac{\partial n_i}{\partial t} + \frac{\partial(n_i u_i)}{\partial x} = S, \quad (3.11)$$

$$\frac{\partial u_i}{\partial t} = -u_i \frac{\partial u_i}{\partial x} + \frac{Ze}{m_i} E + \frac{R_{ie} + R_{CX}}{m_i n_i} - \frac{S}{n_i} u_i - \frac{1}{m_i n_i} \frac{\partial(n_i kT_i)}{\partial x}. \quad (3.12)$$

In equation 3.12 there are two friction terms, where  $R_{ie}$  is obtained by requiring total momentum in electron-ion collisions to be conserved, thus  $R_{ie} = -R_{ei}$ . The second friction term  $R_{CX}$  is a simple charge exchange friction term, given by

$$R_{CX} = -n_i m_i u_i |u_i| \sum_b n_b \sigma_{CX,b}, \quad (3.13)$$

where the sum is over neutral atomic states, and both the ions and neutrals are approximated as cold (with no neutral flow), and the simplified constant charge exchange cross sections are given by approximate low energy values for hydrogen obtained from Janev[55]

$$\sigma_{CX,1} = 3 \times 10^{-19} m^2, \quad \sigma_{CX,2} = 2^4 \times 10^{-19} m^2, \quad \sigma_{CX,3} = 3^4 \times 7 \times 10^{-20} m^2, \quad \sigma_{CX,b \geq 4} = b^4 \times 6 \times 10^{-20} m^2.$$

To calculate the electric field, Ampère-Maxwell's law is solved, which contains only the displacement current, due to the parallel nature of the problem

$$\frac{\partial E}{\partial t} = -\frac{1}{\epsilon_0}(j_e + Zen_i u_i), \quad (3.14)$$

where  $j_e$  is either given as a moment of the electron distribution function, or simply as  $j_e = -en_e u_e$  in the electron fluid case. Allowing the field to evolve in this way, and keeping the option to solve the continuity equation for ions as well as that for the electrons, makes it possible to resolve physics on time and space scales where quasi-neutrality is not observed. While this is not utilised in the work presented, it should in principle extend the application range of the model into highly collisionless regimes.

Allowing the ions to flow, together with solving Ampère-Maxwell's law, lets electrons flow as well. This becomes important as the boundary acts as a sink of particles, while ionisation acts as a source, and flow is necessary in order to avoid nonphysical local depletion/overflow of electron/ion density.

At the sheath boundary, ions reach the sound speed. In both the fluid and kinetic case, ambipolar flux is assumed, and in the fluid mode the sheath heat transmission coefficient in the transmitted sheath heat flux (equation (2.12)) is set to  $\gamma_e = 2 - 0.5 \ln(2\pi(1 + T_i/T_e)m_e/m_i)$ [12].

### 3.3 Diffusive-Reactive Collisional-Radiative model

In order to accurately model the interaction of the plasma with the atomic hydrogen/deuterium, it is necessary to perform some sort of tracking of the various atomic states. This can be done using a diffusive-reactive collisional-radiative model (CRM)[97]

$$\begin{aligned}
 \frac{\partial n_b}{\partial t} = & \frac{\partial}{\partial x} \left( D_b \frac{\partial n_b}{\partial x} \right) + \sum_{b' < b} [K_{b' \rightarrow b}^e n_{b'} - A_{b \rightarrow b'} n_b - K_{b \rightarrow b'}^e n_b] \\
 & + \sum_{b' > b} [K_{b' \rightarrow b}^e n_{b'} + A_{b' \rightarrow b} n_{b'} - K_{b \rightarrow b'}^e n_b] - K_b^{ion} n_b + \alpha_b n_e^2 n_i + \beta_b n_e n_i.
 \end{aligned} \tag{3.15}$$

The model above includes all of the collisional and radiative atomic processes treated in SOL-KiT.

These are the following:

- Collisional excitation and deexcitation - these are transitions between states  $b$  and  $b'$  induced by electron impact, and where the rates are labeled by  $K^e$
- Radiative deexcitation/Spontaneous emission - transition rates labeled by  $A$
- Electron impact ionisation - with rates  $K^{ion}$
- Radiative recombination - recombination resulting in a photon with the ionisation energy, with rates  $\beta$
- Three-body recombination - inverse process to electron impact ionisation, rates labeled by  $\alpha$
- Diffusion governed by elastic and charge exchange collisions - with diffusion coefficient  $D$

The calculation of ionisation and (de)excitation rates  $K$ , as well as three-body recombination rates  $\alpha$  are performed using moments of the distribution function (see section 3.4). Inelastic cross-sections and radiative deexcitation/recombination rates  $A$  and  $\beta$  are all taken from Janev[55] and NIST[98]. At present, radiative deexcitation rates are included up to state  $n = 20$ , due to lack of available data. However, since higher excited states are primarily collisionally coupled in most situations of interest this should not cause significant discrepancies.

The classical 1D diffusion coefficient is given simply by

$$D_b = \frac{v_{tn}}{2[(n_i + n_1)\sigma_{el} + \sigma_{CX,b}n_i]} \tag{3.16}$$

where  $v_{tn} = (2kT_n/m_n)^{1/2}$  is the thermal speed of neutrals, and  $\sigma_{el}$  is the elastic collision cross-section (see electron-neutral elastic collision operator in 3.4), and  $n_1$  is the ground state density. When charge exchange is used, it is the dominant term in the diffusion coefficient, but the elastic collision diffusion is included for cases when charge exchange is not used. The neutral mass can be taken to be equal to that of the ions  $m_n = m_i$ , while the neutral temperature  $T_n$  is a free parameter of the model.

Finally, the atomic neutrals are recycled with a recycling flux  $\Gamma_{REC} = -R\Gamma_i$ , where  $R \leq 1$  is the recycling coefficient. This is imposed by setting  $D_1\partial n_1/\partial x$  in (3.15) at the boundary to  $\Gamma_{REC}$ , thus recycling all neutrals into the ground state. For  $b > 1$  the divertor boundary condition  $D_b\partial n_b/\partial x = 0$  is imposed. At the upstream boundary the neutral flux for all states is set to zero, though the neutral number density at  $x = 0$  is generally negligible.

### 3.4 The Legendre decomposition of the electron kinetic equation

Due to the great mass difference between electrons and other species within a hydrogen plasma, electrons mainly suffer pitch-angle scattering collisions when colliding with those heavier particles. Eigenfunctions of the pitch-angle scattering operator are spherical harmonics, and an expansion of the electron distribution function in spherical harmonics becomes natural[99]. This approach has been used in the modeling of Scrape-Off-Layer transport to a limited extent[72, 70, 3](as was covered in the previous chapter), but has been used both in codes dealing with laser-plasma interactions (KALOS[100]/OSHUN[101], and IMPACT[102]), as well as electron swarm transport models[103, 104]. The expansion has been used to efficiently model both Coulomb and electron-neutral collisions, and has proven itself to be a powerful tool in treating plasmas of various collisionality. With this in mind, a marriage of the Vlasov-Fokker-Planck approach in laser plasmas and the Boltzmann approach of electron swarms in neutral gases seems to be potentially a highly applicable model for the Scrape-Off Layer plasma, where collisionality changes, and plasma-neutral interactions carry a great deal of importance.

Spherical harmonics are an orthonormal basis set in the solid angle space  $(\theta, \varphi) \in [0, \pi) \times$

$[0, 2\pi)$ [105], and can be written as a suitably normalised product of associated Legendre polynomials  $P_l^m(\cos \theta)$  and the complex phase  $e^{im\varphi}$ . The spherical harmonic convention used in SOL-KiT is same as the ones in KALOS[100]/OSHUN[101]. As such, the traditional Cartesian coordinate system for velocity  $(v_x, v_y, v_z)$  will be rotated so that the angles  $\theta$  and  $\varphi$  are defined as part of a spherical coordinate system:

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}, \quad \theta = \arccos(v_z/v), \quad \varphi = \arctan(v_y/v_x). \quad (3.17)$$

If the distribution function  $f(v, \theta, \phi)$  is then decomposed in spherical harmonics, that decomposition is as follows

$$f(v, \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l f_l^m(v) P_l^{|m|}(\cos \theta) e^{im\varphi} \quad (3.18)$$

where the complex expansion coefficients  $f_l^m$  satisfy  $(f_l^m)^* = f_l^{-m}$ . This allows writing the kinetic equation for electrons as a set of equations for the amplitudes  $f_l^m$ , whose physical significance becomes obvious when moments of the distribution function are expressed using the expansion. If  $\phi$  is a scalar function of  $v$  then

$$\int \phi f(\vec{v}) d\vec{v} = 4\pi \int_0^{\infty} \phi f_0^0(v) v^2 dv \quad (3.19)$$

while if  $\vec{a}$  is a vector function of  $v$

$$\int \vec{a} f(\vec{v}) d\vec{v} = \frac{4\pi}{3} \int_0^{\infty} \|\vec{a}\| \begin{pmatrix} f_1^0 \\ 2\text{Re}(f_1^1) \\ -2\text{Im}(f_1^1) \end{pmatrix} v^2 dv \quad (3.20)$$

and similarly for higher order tensor moments[99, 101]. As can be seen from this, not only does the spherical harmonic expansion have useful properties in relation to collisions, it also provides a physically meaningful decomposition for evaluating transport quantities. For example, density and energy, as scalar quantities are moments of  $f_0^0$ , while the flow velocity and the heat flux are vector quantities and thus moments of  $f_1^m$ .

As azimuthal symmetry around the  $x$ -axis is assumed, and magnetic field effects are ignored,

the spherical harmonic decomposition reduces to a Legendre polynomial decomposition ( $m = 0$  always). Accordingly, harmonics will be labeled only by their  $l$ -number throughout the rest of this text, i.e.  $f_l(v)$ . To obtain the Legendre harmonics  $f_l(v)$  from a given  $f(v, \theta)$  (note that  $\varphi$  dependence is dropped due to symmetry), the Legendre polynomial  $P_l(\cos \theta)$  orthogonality relation (see Appendix C) is used, giving

$$f_l(v) = \frac{2l+1}{2} \int_0^\pi f(v, \theta) P_l(\cos \theta) \sin \theta d\theta. \quad (3.21)$$

Following the Legendre decomposition of the distribution function as outlined above, the 1D kinetic equation can be written as a set of equations

$$\frac{\partial f_l(x, v, t)}{\partial t} = A_l + E_l + C_l, \quad (3.22)$$

where now all of the operators are moved to the RHS and are functions of  $l$  in addition to whatever arguments they naturally have. These will be examined in detail below.

### 3.4.1 Vlasov terms

The two Vlasov terms in equation (3.22) are the spatial advection term  $A_l$  (corresponding to the second LHS term in (3.1)), and the velocity space advection term due to the electric field in the  $x$ -direction  $E_l$  (corresponding to the third LHS term in (3.1)).

Firstly, the spatial advection term (advection in the  $x$ -direction), for a given harmonic  $l$  is

$$A_l = -\frac{l}{2l-1} v \frac{\partial f_{l-1}}{\partial x} - \frac{l+1}{2l+3} v \frac{\partial f_{l+1}}{\partial x}. \quad (3.23)$$

Spatial advection couples harmonics with different  $l$  numbers. The physical significance of this coupling is most easily seen in the coupling between  $f_0$  and  $f_1$ . As noted above, moments of  $f_0$  are the density and total energy, while  $f_1$  is associated with flows (of particles and energy). Thus gradients in  $f_0$  (density and temperature) drive  $f_1$  (flows), and vice-versa, as expected from a fluid point of view.

The velocity space advection term due to the electric field couples harmonics as well, albeit

through velocity space gradients in  $f_l$ . As only the  $x$  component of the electric field is treated, in the remainder of the text it will simply be written as  $E$  for brevity. The velocity space advection operator is given by [100]

$$E_l = \frac{e}{m} E \left[ \frac{l}{2l-1} G_{l-1} + \frac{l+1}{2l+3} H_{l+1} \right] \quad (3.24)$$

where

$$G_l(v) = v^l \frac{\partial v^{-l} f_l}{\partial v}, \quad (3.25)$$

$$H_l(v) = \frac{1}{v^{l+1}} \frac{\partial v^{l+1} f_l}{\partial v}. \quad (3.26)$$

As is evident from equation (3.24), the electric field couples harmonics through the  $G_l$  and  $H_l$  functions, which contain velocity space gradients of the coupled harmonics.

Thus, Vlasov terms provide coupling of harmonics through either spatial gradients or the electric field.

### 3.4.2 Coulomb collision terms

Consider the effect of Coulomb collisions on the distribution function  $f$  of particles of mass  $m$  and charge  $q = ze$  colliding with particles of mass  $M = \mu_r m$  and charge  $Q = Ze$  with distribution  $F$ . Note that  $\mu_r$  is the mass ratio, not to be confused with the reduced mass  $\mu$  from the previous chapter. Following the formalism of Shakorfsky et al. [99], the Rosenbluth coefficient formulation of the Fokker-Planck collision operator for Coulomb collisions

$$\frac{1}{\Gamma_{zZ}} \frac{\delta f}{\delta t} = \frac{4\pi}{\mu_r} F f + \frac{\mu_r - 1}{\mu_r + 1} \nabla \mathcal{H}(F) \cdot \nabla f + \frac{\nabla \nabla \mathcal{G}(F) : \nabla \nabla f}{2}, \quad (3.27)$$

is used as a starting point, where  $\nabla = \partial/\partial \vec{v}$  and  $\Gamma_{zZ} = (zZe^2)^2 \ln \Lambda / (4\pi(m\epsilon_0)^2)$ , with  $\ln \Lambda$  denoting the Coulomb logarithm. The Rosenbluth drag and diffusion coefficients are respectively  $\mathcal{H}$  and  $\mathcal{G}$ . The distribution functions are separated into their isotropic and anisotropic components  $F = F_0 + F_a$ ,  $f = f_0 + f_a$ . The key assumption going forward is that the anisotropic component

is small compared to the isotropic one, so that it becomes possible to linearise equation (3.27). Expanding the distribution function and the Rosenbluth coefficients in harmonics and using the integrals[99]

$$I_j(F_l) = \frac{4\pi}{v^j} \int_0^v F_l(u) u^{j+2} du, \quad J_j(F_l) = \frac{4\pi}{v^j} \int_v^\infty F_l(u) u^{j+2} du, \quad (3.28)$$

one can derive the expressions for the harmonic components of the Fokker-Planck collision integral for all  $l$ . For  $l = 0$  this is

$$\frac{1}{\Gamma_{ZZ}} \frac{\delta f_0}{\delta t} = \frac{1}{3v^2} \frac{\partial}{\partial v} \left[ \frac{3}{\mu_r} f_0 I_0(F_0) + v (I_2(F_0) + J_{-1}(F_0)) \frac{\partial f_0}{\partial v} \right]. \quad (3.29)$$

For  $l > 0$  the following is obtained[101]

$$\begin{aligned} \frac{1}{\Gamma_{ZZ}} \frac{\partial f_l}{\partial t} = & \frac{4\pi}{\mu_r} [F_0 f_l + f_0 F_l] \\ & - \frac{(\mu_r - 1)}{\mu_r v^2} \left\{ \frac{\partial f_0}{\partial v} \left[ \frac{l+1}{2l+1} I_l(F_l) - \frac{l}{2l+1} J_{-1-l}(F_l) \right] + I_0(F_0) \frac{\partial f_l}{\partial v} \right\} \\ & + \frac{I_2(F_0) + J_{-1}(F_0)}{3v} \frac{\partial^2 f_l}{\partial v^2} + \frac{-I_2(F_0) + 2J_{-1}(F_0) + 3I_0(F_0)}{3v^2} \frac{\partial f_l}{\partial v} \\ & - \frac{l(l+1)}{2} \times \frac{-I_2(F_0) + 2J_{-1}(F_0) + 3I_0(F_0)}{3v^3} f_l \\ & + \frac{1}{2v} \frac{\partial^2 f_0}{\partial v^2} [C_1 I_{l+2}(F_l) + C_1 J_{-1-l}(F_l) + C_2 I_l(F_l) + C_2 J_{1-l}(F_l)] \\ & + \frac{1}{v^2} \frac{\partial f_0}{\partial v} [C_3 I_{l+2}(F_l) + C_4 J_{-1-l}(F_l) + C_5 I_l(F_l) + C_6 J_{1-l}(F_l)], \end{aligned} \quad (3.30)$$

where the  $C$  coefficients are functions of  $l$

$$\begin{aligned} C_1 &= \frac{(l+1)(l+2)}{(2l+1)(2l+3)}, \quad C_2 = -\frac{(l-1)l}{(2l+1)(2l-1)}, \quad C_3 = -\frac{(l+1)l/2 + l + 1}{(2l+1)(2l+3)}, \\ C_4 &= \frac{-(l+1)l/2 + l + 2}{(2l+1)(2l+3)}, \quad C_5 = \frac{(l+1)l/2 + l - 1}{(2l+1)(2l-1)}, \quad C_6 = -\frac{(l+1)l/2 - l}{(2l+1)(2l-1)}. \end{aligned}$$

For electron-electron collisions  $\mu_r = 1$ . The effect of e-e collisions on the isotropic part of the distribution function  $f_0$  is given by

$$\frac{1}{\Gamma_{ee}} \left( \frac{\delta f_0}{\delta t} \right)_{e-e} = \frac{1}{v^2} \frac{\partial}{\partial v} \left[ C(f_0) f_0 + D(f_0) \frac{\partial f_0}{\partial v} \right], \quad (3.31)$$

where the drag and diffusion coefficients are defined as

$$C(f_0) = 4\pi \int_0^v f_0(u) u^2 du, \quad (3.32)$$

$$D(f_0) = 4\pi \int_0^v u^2 \left[ \int_u^\infty f_0(u') u' du' \right] du. \quad (3.33)$$

Note that  $D$  is not in the form one would expect from equation (3.29). Instead, it is written in an analytically equivalent form (see Section 4.5). The electron-electron collision operator for  $l = 0$  is important for the proper relaxation of the electron distribution function to a Maxwellian.

For higher harmonics, from (3.30) one gets

$$\begin{aligned} \frac{1}{\Gamma_{ee}} \left( \frac{\delta f_l}{\delta t} \right)_{e-e} &= 8\pi f_0 f_l + \frac{I_2(f_0) + J_{-1}(f_0)}{3v} \frac{\partial^2 f_l}{\partial v^2} \\ &+ \frac{-I_2(f_0) + 2J_{-1}(f_0) + 3I_0(f_0)}{3v^2} \frac{\partial f_l}{\partial v} \\ &- \frac{l(l+1)}{2} \times \frac{-I_2(f_0) + 2J_{-1}(f_0) + 3I_0(f_0)}{3v^3} f_l \\ &+ \frac{1}{2v} \frac{\partial^2 f_0}{\partial v^2} [C_1 I_{l+2}(f_l) + C_1 J_{-l-1}(f_l) + C_2 I_l(f_l) + C_2 J_{1-l}(f_l)] \\ &+ \frac{1}{v^2} \frac{\partial f_0}{\partial v} [C_3 I_{l+2}(f_l) + C_4 J_{-l-1}(f_l) + C_5 I_l(f_l) + C_6 J_{1-l}(f_l)]. \end{aligned} \quad (3.34)$$

As the ions are either assumed cold or with the same temperature as the electrons, in the current version of SOL-KiT the effect of electron-ion collisions on  $f_0$  is not included. The effect of such an operator would be the exchange of energy between ions and electrons, with the equilibrium distribution (in absence of driving forces) being a Maxwellian of the ion temperature  $T_i$ . Note, however, that this operator would be of order  $O(m_e/m_i)$ .

For higher harmonics two cases of electron-ion collisions are distinguished in the model. The first is the classical stationary ion case, where  $F_0 = n_i \delta(v)/(4\pi v^2)$ . It can easily be shown that equation (3.30) reduces to the following eigenfunction form

$$\left(\frac{\delta f_l}{\delta t}\right)_{e-i} = -\frac{l(l+1)}{2} \frac{\Gamma_{ei} n_i}{v^3} f_l. \quad (3.35)$$

This is purely angular scattering, which dampens higher harmonics, allowing natural truncation of the expansion.

However, when ions are not stationary, but are moving at some velocity much smaller than the electron thermal velocity (the case expected in the SOL), it is necessary to modify the electron-ion collision operator. As was noted in the previous chapter, flows in the SOL are induced by the presence of the sheath boundary condition[12], and this requires the treatment of the ions in the lab frame in order to define the ambipolar flow in the logical boundary condition[69](see 3.5). The usual approach in Legendre decomposition methods is to move into the ion rest frame, allowing the stationary ion treatment of the electron-ion collision operator[106, 107]. Moving into the ion rest frame pushes all of the complexity into the Vlasov terms, i.e. the LHS of the kinetic equation. However, due to the above constraint with the logical boundary condition, the electron-ion collision operator must be dealt with in the lab frame, and, contrary to the standard approach, it must carry the complexity of including ion flows instead of the Vlasov terms. The first step in including ion flow effects in the collision operator is the removal of all the terms proportional to the inverse mass ratio in equation (3.30). To calculate the  $I$  and  $J$  integrals for a cold ion stream let the ion distribution function be

$$F(\vec{v}) = n_i \delta(\vec{v} - \vec{u}_i) \quad (3.36)$$

Recasting the Dirac delta into spherical coordinates assuming azimuthal symmetry and expanding in Legendre polynomials gives us

$$F_l(v) = \frac{n_i(2l+1)}{4\pi v^2} \delta(v - u_i). \quad (3.37)$$

Substituting these harmonics into the equations for the  $I$  and  $J$  integrals gives

$$I_j(F_l) = (2l+1)n_i \frac{u_i^j}{v^j} \Theta(v - u_i), \quad (3.38)$$

$$J_j(F_l) = (2l + 1)n_i \frac{u_i^j}{v^j} \Theta(u_i - v), \quad (3.39)$$

where  $\Theta$  denotes the Heaviside step function. It is now trivial to see that all but the  $I_0$  integrals vanish when  $u_i = 0$ , recovering the stationary ion collision integral. It can also be easily shown that for small enough  $u_i$ , the collision integral for  $f_1$  reduces to [99]

$$\frac{1}{\Gamma_{ZZ}} \frac{\partial f_1}{\partial t} = -\frac{n_i}{v^3} \left( f_1 + u_i \frac{\partial f_0}{\partial v} \right). \quad (3.40)$$

If  $f_0$  is taken to be Maxwellian, this gives a stationary solution to the  $f_1$  collision operator to be that  $f_1$  which yields a slowly drifting Maxwellian with drift velocity  $u_i$ .

Taking a closer look at the obtained collision integral, it can be seen that electrons slower than the ions are being carried around by them, as one would expect. This modifies all harmonics for small  $v$ , so the convenient property of clean truncation of the distribution function by electron-ion collisions is lost. However, in realistic simulation cases, this happens only for a small handful of velocity space cells, while higher harmonics are normally dampened in the rest of velocity space. This is to be expected, as electrons see an ion Dirac delta and are collisionally driven towards it.

### 3.4.3 Boltzmann collision terms

The implementation of electron-neutral collisions starts from the general form of the Boltzmann collision integral for the effect of collisions on the distribution function of species  $s$  colliding with species  $s'$

$$C[f_s, f_{s'}](v) = \int d\vec{v}_2 d\Omega |\vec{v} - \vec{v}_2| \sigma(|\vec{v} - \vec{v}_2|, \Omega) [f_s(\vec{v}') f_{s'}(\vec{v}_2') - f_s(\vec{v}) f_{s'}(\vec{v}_2)], \quad (3.41)$$

where primed velocities denote values before a collision, and  $\sigma$  is the appropriate differential cross-section, as was covered in the previous chapter. The following results are all derived under the assumption of a small mass ratio and stationary (slow compared to the electrons) neutral particles (atoms) [99, 103, 104]. Furthermore, all differential cross-sections are assumed to be

azimuthally symmetric, i.e. are only the function of energy/velocity of the impacting particle (electron), and the deflection angle (here  $\chi$ ). This just means that the cross-sections do not depend on the orientation of the neutral particle.

**Elastic electron-neutral collisions** The first term in the small mass expansion of the electron-neutral elastic collision integral cancels for  $l = 0$ . It is therefore necessary to include higher order effects of collisional energy transfer. This way, one can allow for long term relaxation of the electron distribution function to a Maxwellian with temperature equal to the gas temperature  $T_g$ . If  $M$  is the neutral mass, and  $n_b$  the gas density, the collision integral takes the form

$$\left(\frac{\delta f_0}{\delta t}\right)_{e-n_b} = \frac{m_e}{M + m_e} \frac{1}{v^2} \frac{\partial}{\partial v} \left[ n_b v^4 \left( \int d\Omega (1 - \cos \chi) \sigma_b^{el}(\chi, v) \right) \left( f_0 + \frac{kT_g}{m_e v} \frac{\partial f_0}{\partial v} \right) \right] \quad (3.42)$$

As is the case with electron-ion Coulomb collisions, due to a great mass difference, the  $l > 0$  integral is considerably simplified, and can be written as

$$\left(\frac{\delta f_{l>0}}{\delta t}\right)_{e-n_b} = -n_b v \left[ \int d\Omega (1 - P_l(\cos(\chi)) \sigma_b^{el}(\chi, v) \right] f_l. \quad (3.43)$$

where  $P_l$  is simply the  $l$ -th Legendre polynomial.

While implemented and tested in the current version of SOL-KiT, these two processes are rarely used, because of the lack of proper elastic collision cross-section data in the model. Currently the cross-section for elastic collisions of an electron with a hydrogen atom in a given state is obtained using the classical expression for orbit size. Namely, this gives for the integral elastic collision cross-section of electrons with hydrogen atoms in the  $b$ -th state

$$\int \sigma_b^{el} d\Omega = \pi a_0^2 b^4 \quad (3.44)$$

where  $a_0$  is the Bohr radius.

**Inelastic electron-neutral collisions** The simplest place to start the description of inelastic collisions is with those where the total number of particles of each species is conserved (e.g. excitation). A standard procedure exists[99, 103] for an inelastic collision for which the pre-collision and post-collision velocities are related as

$$\frac{m_e v'^2}{2} = \frac{m_e v^2}{2} + \epsilon \quad (3.45)$$

where  $\epsilon$  is the inelastic energy loss. Note that interchanging the pre-and post-collision velocities when talking about inelastic collisions is not possible without changing the sign of  $\epsilon$ , contrary to elastic collisions. Defining  $\alpha = v'/v = (1 + 2\epsilon/mv^2)^{1/2}$ , one can write the collision integral as

$$\left( \frac{\delta f_l}{\delta t} \right)_{b \rightarrow b'}^{ex} = -n_b v \left[ \sigma_{b \rightarrow b'}^{TOT}(v) f_l(v) - f_l(\alpha v) \alpha^2 \left( \sigma_{b \rightarrow b'}^{TOT}(\alpha v) - \sigma_{b \rightarrow b'}^{(l)}(\alpha v) \right) \right]. \quad (3.46)$$

Here  $\sigma^{TOT} = \int d\Omega \sigma(\chi, v)$  is the integral cross section, while

$$\sigma^{(l)}(v) = \int d\Omega (1 - P_l(\cos \chi)) \sigma(\chi, v).$$

Using equation (3.46) for  $l = 0$  one can easily show that particle number is conserved.

On the other hand, collisional processes such as ionisation do not conserve the total number of particles. The main difficulty in treating ionisation is the fact that it is, ultimately, a 3-body process, and ideally one would like to know the triply differential cross section for such a process. However, such an approach is not only complicated, but cross-section data (to the author's knowledge) are not systematically available. Because of this, the approach taken here will be the simplest possible[2], where all electrons produced through ionisation are put in the lowest velocity cell, while the original electron experiences a standard energy loss/deflection as in the case of excitation. The collisional operator for ionisation takes the following form

$$\left( \frac{\delta f_l}{\delta t} \right)_b^{ion} = \left( \frac{\delta f_l}{\delta t} \right)^{ex} (\sigma_b^{ion}) + n_b K_b^{ion} \frac{\delta(v)}{4\pi v^2} \delta_{l,0} \quad (3.47)$$

where  $\left( \frac{\delta f_l}{\delta t} \right)^{ex} (\sigma_b^{ion})$  is equation 3.46, but with  $\sigma^{ex}$  replaced with  $\sigma^{ion}$ , with the collisional ionisation rate coefficient defined (unconventionally) as

$$K_b^{ion} = 4\pi \int dv v^3 f_0(v) \sigma_b^{TOT,ion}(v). \quad (3.48)$$

Particle sources are then computed using  $S_{ion} = \sum_b K_b^{ion} n_b$ , and similarly for recombination. Any collisional transition rate can be written in the same way as the above, with the only difference being the cross-section. The inelastic collision contribution to the heating term  $Q = Q_{ext} + Q_{en}$  in the fluid electron temperature equation (3.7) is calculated by taking the product of each transition rate and the associated transition energy, i.e.

$$Q_{en} = - \sum_{b,b'} K_{b \rightarrow b'} n_b \epsilon_{b \rightarrow b'}, \quad (3.49)$$

where the sum is over all atomic states, including the ionised state. The above sum is a shorthand for all of the relevant collisional processes in equation (3.15), where  $\epsilon_{b \rightarrow b'}$  is the transition energy (e.g. excitation or ionisation energy).

Inverse processes (deexcitation and 3-body recombination) are treated using the principle of detailed balance [108, 109] to obtain cross-sections. The principle of detailed balance states that in local thermodynamic equilibrium each process is balanced exactly by its inverse. For deexcitation, this gives

$$\sigma_{deex}(i, j, v') = \frac{g_j}{g_i} \frac{v^2}{v'^2} \sigma_{ex}(j, i, v) \quad (3.50)$$

where  $i$  and  $j$  are atomic states ( $j < i$ ), and  $g_i$  and  $g_j$  their statistical weights. For hydrogen these are simply  $g_n = 2n^2$ . Equation (3.45) defines the velocities, but a negative  $\epsilon$  is used.

For 3-body recombination, using the statistical weights of a free electron gas the following is obtained

$$\sigma_{3b-recomb}(i, v') \frac{1}{n_e} = \frac{g_i}{2g_1^+} \left( \frac{h^2}{2\pi m_e k T_e} \right)^{3/2} \times \frac{v^2}{v'^2} \sigma_{ion}(i, v), \quad (3.51)$$

where  $h$  is the Planck constant,  $n_e$  and  $T_e$  are the electron density and temperature, respectively, and  $g_1^+$  is the ion ground state statistical weight (for hydrogen simply  $g_1^+ = 1$ ).

To calculate the electron fluid mode friction with the neutrals  $R_{en}$  in equation (3.3) terms of

the following form are used

$$R_{en}^{ion} = \sum_b \frac{4\pi}{3} \int_0^\infty m_e \left( \frac{\delta f_1}{\delta t} \right)_b^{ion} v^3 dv, \quad (3.52)$$

where  $f_1(v) = -u_e \partial f_0 / \partial v$  (with Maxwellian  $f_0$ ), and similarly for other neutral processes. Summing over all processes and atomic states results in the total friction experienced by the electrons due to electron-neutral collisions.

### 3.4.4 Source operators for the $f_0$ equation

In order to emulate external heating and particle sources a number of operators are included in the model. Conveniently, energy and particles are governed by the  $f_0$  equation, so as long as the sources are isotropic they act only on the  $l = 0$  harmonic.

#### Electron heating operator

The simplest way to implement a heating operator is with a diffusive model

$$\left( \frac{\partial f_0}{\partial t} \right)_{heating} = \Theta(L_h - x) D(x, t) \frac{1}{3v^2} \frac{\partial}{\partial v} v^2 \frac{\partial f_0}{\partial v}, \quad (3.53)$$

where  $\Theta(L_h - x)$  is the step function designating the heating region upstream. It is easy to show that this operator conserves particle number if  $v^2 \partial f_0 / \partial v = 0$  on the system boundaries ( $v = 0$  and  $v \rightarrow \infty$ ). If spatially uniform heating is assumed, it can be shown that

$$D(x, t) = \frac{W_h(t)}{m_e n_e(x, t) L_h}, \quad (3.54)$$

where  $W_h(t)$  is the heat flux entering the SOL over length  $L_h$ . This is related to the fluid model heating  $Q_{ext}$  via  $Q_{ext} = W_h / L_h$ .

#### Particle source operator

In order to treat upstream density perturbations, the following electron and ion particle sources are included in the model when simulating kinetic electrons

$$\left(\frac{\partial f_0}{\partial t}\right)_{source} = \Theta(L_s - x)F_R(x, t) \left(\frac{m_e}{2\pi k T_{source}}\right)^{3/2} e^{\frac{-mv^2}{2k T_{source}}}, \quad (3.55)$$

where  $F_R$  is the source rate coefficient

$$F_R = \frac{\Gamma_{in}}{L_s}, \quad (3.56)$$

with  $\Gamma_{in}$  being the effective upstream flux. The particles are injected over a length of  $L_s$  and with temperature  $T_{source}$ , which can be the background temperature.

The ion particle source is simply

$$\left(\frac{\partial n_i}{\partial t}\right)_{source} = \Theta(L_s - x)F_R. \quad (3.57)$$

### 3.5 The logical boundary condition in the Legendre formalism

At the divertor target, electrons which have enough energy to overcome the sheath potential are lost to the material surface, while all others are reflected. When combined with the condition that flow is ambipolar ( $n_e u_e = n_i u_i$ ) at the sheath entrance, this becomes the standard logical boundary condition [69]. Effectively, the electron distribution function has a sharp cut-off at some parallel velocity  $-v_c$  (where  $v_c$  is defined as positive) representing the lost electrons. The challenge when formulating this condition in a Legendre polynomial formalism is the extreme anisotropy that results from it, which would require a high number of harmonics to resolve to a satisfactory level. Fortunately, in practice this number is usually not prohibitively high (see benchmarking in next chapter). In this section the newly developed logical boundary condition formulated using Legendre polynomials is presented.

The first step is to construct the distribution function before decomposing it into harmonics. Assuming the distribution function for positive  $v_x$  (moving towards the divertor target) is known it can be expanded into Legendre polynomials (assuming azimuthal symmetry, of course)

$$f(v_x > 0, v_\perp) = \sum_l f_l(v) P_l(\cos \theta), \quad \cos \theta > 0,$$

where  $v_\perp$  denotes the velocity in the direction perpendicular to the magnetic field, i.e. to the  $x$ -axis. If all electrons were to be reflected, the total (reflection included) distribution function would be

$$f_R(v, \theta) = \sum_l f_l(v) P_l(|\cos \theta|).$$

Finally, all of the electrons that would have been lost to the sheath and thus should not be in the distribution function are removed. This is simply all electrons with  $v \cos \theta = v_x < -v_c$ . Using a Heaviside step function, this can be expressed as

$$f_c(v, \theta) = f_R(v, \theta) \Theta(v \cos \theta + v_c). \quad (3.58)$$

From here the Legendre polynomial orthogonality relation (see Appendix C) is used to extract the  $l$ -th harmonic of the “cut-off” distribution

$$f_{cl}(v) = \frac{2l+1}{2} \int_{-1}^1 f_R(v, \theta) \Theta(v \cos \theta + v_c) P_l(\cos \theta) d(\cos \theta). \quad (3.59)$$

Using the decomposition of  $f_R$ , equation (3.59) becomes

$$f_{cl}(v) = \frac{2l+1}{2} \sum_{l'} f_{l'}(v) \int_{-1}^1 P_{l'}(|\cos \theta|) P_l(\cos \theta) \Theta(v \cos \theta + v_c) d(\cos \theta). \quad (3.60)$$

Here it is helpful to visualise the two-dimensional velocity space of the cut-off. This is shown in Fig 3.2. As can be seen, the integral in (3.60) has different limits depending on the value of the velocity  $v$ . This can be written as (taking  $x = \cos \theta$ )

$$f_{cl}(v) = \frac{2l+1}{2} \sum_{l'} f_{l'}(v) \int_{x_{min}}^1 P_{l'}(|x|) P_l(x) dx, \quad (3.61)$$

where  $x_{min} = \max(-1, \cos \theta_{max}(v))$ , with  $\cos \theta_{max} = -v_c/v$ . Introducing the transformation matrix  $P_{ll'}$  ( $v$  dependence implied)

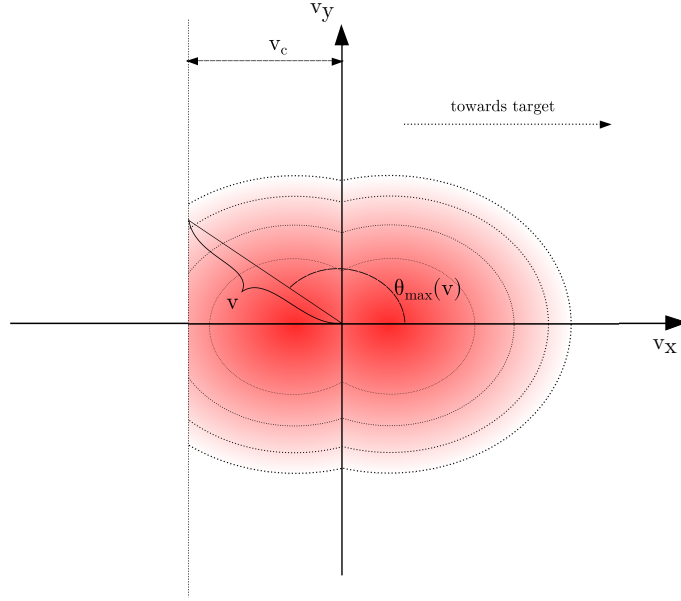


Figure 3.2: The distribution function (anisotropy exaggerated) after applying reflection and cut-off. Highlighted is the angle integration limit  $\theta_{\max}(v)$ .

$$P_{ll'} = \frac{2l+1}{2} \int_{x_{\min}}^1 P_{l'}(|x|) P_l(x) dx, \quad (3.62)$$

a compact expression for the sheath edge electron distribution harmonics results

$$f_{cl}(v) = \sum_{l'} P_{ll'} f_{l'}(v). \quad (3.63)$$

Now the problem is reduced to computing the matrix  $P_{ll'}$ . Separating the integral into positive and negative  $x$  intervals disposes of the absolute value in the argument of  $P_{l'}$

$$P_{ll'} = \frac{2l+1}{2} \left( (-1)^{l'} \int_{x_{\min}}^0 P_{l'}(x) P_l(x) dx + \int_0^1 P_{l'}(x) P_l(x) dx \right), \quad (3.64)$$

where the parity property of Legendre polynomials  $P_l(-x) = (-1)^l P_l(x)$  was used. In order to reduce the integrals in (3.64) to forms available in the literature the integration range is expanded in the first integral up to 1 and after grouping terms up, the following form is obtained

$$P_{ll'} = P_{ll'}^x + P_{ll'}^0, \quad (3.65)$$

where

$$P_{ll'}^x = \frac{2l+1}{2}(-1)^{l'} \int_{x_{min}}^1 P_{l'}(x)P_l(x)dx, \quad (3.66)$$

$$P_{ll'}^0 = \frac{2l+1}{2}(1 - (-1)^{l'}) \int_0^1 P_{l'}(x)P_l(x)dx. \quad (3.67)$$

The integral in (3.66) can be found in the literature (see for example [110] for general case) and well known recurrence formulae for the derivatives of Legendre polynomials (Appendix C) can be used to get

$$P_{ll'}^x = \begin{cases} (-1)^{l'} \delta_{ll'} & \text{if } x_{min} = -1 \\ F_{ll'} & \text{if } x_{min} > -1 \text{ and } l \neq l' \\ F_{ll} & \text{if } x_{min} > -1 \text{ and } l = l' \end{cases}$$

where

$$\begin{aligned} F_{ll'} &= (-1)^{l'} \frac{2l+1}{2} \left[ -\frac{x_{min}}{l+l'+1} P_l(x_{min})P_{l'}(x_{min}) \right. \\ &\quad \left. + \frac{1}{(l-l')(l+l'+1)} (lP_{l-1}(x_{min})P_{l'}(x_{min}) - l'P_l(x_{min})P_{l'-1}(x_{min})) \right], \end{aligned}$$

and

$$F_{ll} = (-1)^l \left[ \frac{1}{2} - \left( \frac{x_{min}}{2} [P_l(x_{min})]^2 + \sum_{k=1}^{l-1} P_k(x_{min})(x_{min}P_k(x_{min}) - P_{k+1}(x_{min})) \right) \right].$$

$P_{ll'}^0$  is given by

$$P_{ll'}^0 = \begin{cases} 0 & \text{if } l' \text{ even} \\ \delta_{ll'} & \text{if } l', l \text{ odd} \\ \frac{2l+1}{(l-l')(l+l'+1)} (lP_{l-1}(0)P_{l'}(0) - l'P_l(0)P_{l'-1}(0)) & \text{if } l' \text{ odd and } l \text{ even} \end{cases}$$

It should be noted that for  $v < v_c$  the above equations give  $P_{ll} = 0$  for all odd  $l$ , which is the consequence of reflection symmetry, from which one can also see that there is no effective flux contribution for  $v < v_c$ .

Knowing the form of the distribution function allows the solving of the ambipolarity condition

$$\frac{4\pi}{3} \int_0^\infty v^3 f_{c1} dv = n_{i,sh} u_{i,sh}, \quad (3.68)$$

where  $n_{i,sh}$  is the extrapolated density at the sheath boundary (see Section 4.7 below), and  $u_{i,sh}$  is the ion velocity at the boundary, given by the Bohm condition [38, 12]

$$u_i \geq c_s = \sqrt{\frac{k(T_e + T_i)}{m_i}}, \quad (3.69)$$

where  $T_e$  is the electron temperature in the last simulation cell, and  $T_i$  is the ion temperature. Solving the ambipolarity condition gives the value of  $v_c$ , and with it the value of the sheath potential drop  $\Delta\Phi = m_e v_c^2 / (2e)$ . The electron distribution harmonics with the correct cut-off velocity can then be used as the dynamically updated boundary condition. If a Maxwellian distribution with zero flow velocity is used as the pre-reflection distribution, the analytical value for the cut-off velocity can be obtained using the above formalism. This is equivalent to solving the following simple integral equation

$$\int_{-v_c}^\infty v_x n_e \left( \frac{m_e}{2\pi k T_e} \right)^{1/2} e^{-m_e v_x^2 / (2k T_e)} dv_x = n_e c_s, \quad (3.70)$$

where the ambipolarity condition was applied with assumed  $Z = 1$  quasineutrality and with  $u_{i,sh} = c_s$ . Solving the above equation for  $v_c$  gives

$$v_c = \sqrt{-\frac{k T_e}{m_e} \ln \left[ 2\pi \frac{m_e}{m_i} \left( 1 + \frac{T_i}{T_e} \right) \right]}, \quad (3.71)$$

which recovers the analytical value of the sheath potential drop [12]

$$\frac{e \Delta\Phi}{k T_e} = -\frac{1}{2} \ln \left[ 2\pi \frac{m_e}{m_i} \left( 1 + \frac{T_i}{T_e} \right) \right]. \quad (3.72)$$

For a deuterium plasma with  $T_e = T_i$ , this is  $\approx 3$ . This implies that the cut-off velocity is

$v_c \approx \sqrt{3}v_{th}$ , where the thermal velocity is defined as  $v_{th} = \sqrt{2kT_e/m_e}$ .

### 3.6 Summary

In order to systematically extract electron kinetic effects in SOL parallel transport, comparison with a fluid model is necessary. A self-consistent fluid and kinetic framework for simulating parallel transport has been presented in this chapter. The fluid model is directly obtained from the moments of the utilised kinetic equation, keeping all of the physics aspects consistent between the two approaches. The full model includes, other than the two electron sets of equations, ion continuity and parallel momentum equations (assuming either  $T_i = 0$  or  $T_i = T_e$ ), a diffusive-reactive Collisional-Radiative model for the atomic neutral states, as well as Ampère-Maxwell’s law for the electric field. Coupling between the different sets of equations is achieved indirectly through the electric field, and directly through various collision operators.

Exploiting the symmetry of collision operators, the choice of Legendre polynomials as a basis was used to rewrite the electron kinetic equation. All kinetic operators are represented in this basis, and instead of solving one electron kinetic equation (1D in space and 2-3D in velocity), a set of equations for the harmonics (1D in space and 1D in velocity) is solved. Collisions provide a natural truncation to the Legendre polynomial expansion, with collisional systems requiring a lower number of harmonics to properly resolve. Both Coulomb and electron-neutral collision operators are included in the model, with Coulomb collisions including electron-electron collisions for all harmonics, and electron-ion collisions for harmonics with  $l > 0$  (i.e. ignoring electron-ion energy exchange).

Since the boundary condition at the divertor target in the SOL acts as a sink of plasma and source of neutrals, a number of additions to the standard Vlasov-Fokker-Planck approach were necessary. Firstly, due to the presence of sinks, ion flows had to be incorporated into the electron-ion collision operator. The neutrals generated through recycling are also tracked in detail and allowed to interact with the electrons through the Boltzmann collision integral. Finally, the standard logical boundary condition for SOL kinetic models [69] had to be formulated in terms of the Legendre polynomial basis.

In the following chapter, the numerics behind the model presented here will be discussed, along with various benchmarking tests of the implemented operators.

# Chapter 4

## Numerics and benchmarking of SOL-KiT

### 4.1 Overview

The numerical implementation of the models presented in the previous chapter is discussed here. After presenting the fundamentals of the grid and normalisation of variables on which the entire code is based, the algorithms and basic discretisation of equations is given. As the novel method for conservative implementation of the inelastic collision operators is a major part of the numerics it is devoted a significant amount of discussion.

A set of benchmarks performed for publication in Computer Physics Communications ends this chapter, with tests that go over all of the major elements of the code.

### 4.2 Normalisation of variables and discretisation of phase space

Variables in the SOL-KiT code are normalised to reference values that capture the basic physics inherent to the SOL. This normalisation will be presented in the following section.

Equations of the various models are all solved on a discrete grid, and the character of that grid is tailored to the problems at hand. Phase space discretisation is presented, going over

variable placement on the spatial grid, and the non-uniform grid options dedicated to the specific problem of strong gradient divertor simulations.

### 4.2.1 Normalisation

To normalise the quantities in SOL-KiT, a reference plasma is used, with a defined temperature (in eV), electron density (in  $m^{-3}$ ), atomic number (assumed to be fully ionised), and atomic mass. These normalisation constants are respectively referred to as  $T_0$ ,  $n_0$ ,  $Z$ , and  $A$ . All other variable normalisations as well as normalisation constants within equations are derived from these four basic reference quantities.

The electron velocity is on the scale of the thermal speed  $v_{th} = (2T_0[J]/m_e)^{1/2}$ , and thus all velocity variables are normalised to  $v_{th}$ . Here  $T_0[J]$  denotes the normalisation temperature converted from eV to Joules. The most important timescale is that of Coulomb collisions, and the chosen time normalisation reflects this. Time is normalised to the  $90^\circ$  electron-ion collision time  $t_0 = v_{th}^3 / (\Gamma_{ei}^0 n_0 \ln \Lambda_{ei}(T_0, n_0) / Z)$ , where

$$\Gamma_{ei}^0 = Z^2 \Gamma_{ee}^0 = Z^2 \frac{e^4}{4\pi(m_e \epsilon_0)^2},$$

and where  $\ln \Lambda_{ei}(T_0, n_0)$  is the Coulomb logarithm for electron-ion collisions calculated for the normalisation temperature and density (taken from [47]). Finally, length is normalised to the thermal electron-ion collision mean free path  $x_0 = v_{th} t_0$ .

All basic normalised quantities are

$$\begin{aligned} \tilde{v} &= \frac{v}{v_{th}}, & \tilde{t} &= \frac{t}{t_0}, & \tilde{x} &= \frac{x}{x_0}, \\ \tilde{f}_l &= \frac{f_l}{n_0 v_{th}^{-3}}, & \tilde{E} &= \frac{E e t_0}{m_e v_{th}}, & \tilde{q} &= \frac{q}{m_e n_0 v_{th}^3}, \\ \tilde{T}_{e,i,g} &= \frac{T_{e,i,g}}{T_0}, & \tilde{n}_{e,i,b} &= \frac{n_{e,i,b}}{n_0}, & \tilde{u}_{e,i} &= \frac{u_{e,i}}{v_{th}}, \\ \tilde{\epsilon} &= \frac{\epsilon}{T_0}, & \tilde{\sigma} &= \frac{\sigma}{\sigma_0}, \end{aligned}$$

where  $\sigma_0 = a_0^2 \pi$  (where  $a_0$  is the Bohr radius). Unless otherwise specified as un-normalised, all

quantities in the following text will be assumed normalised, and the tilde will be dropped.

### 4.2.2 Grids

The electron distribution function harmonics  $f_l$  are resolved on a geometric velocity grid consisting of  $N_v$  cells, with starting width  $\Delta v_1$  and width multiplier  $c_v$ , distributed as

$$v_1 = \frac{\Delta v_1}{2}, \quad \Delta v_n = c_v \Delta v_{n-1}, \quad v_n = v_{n-1} + \frac{1}{2} (\Delta v_n + \Delta v_{n-1}).$$

Using a geometric grid with  $c_v > 1$  allows both resolving in detail the low energy electrons involved in collisions, as well as the high energy collisionless tail. The special case of a uniform velocity grid is recovered by setting  $c_v = 1$ .

All quantities are defined on a staggered spatial grid, consisting of cell centres and boundaries. The number of cell centres (cells) is  $N_c$ , while  $N_x$  is used to denote the total number of spatial points (cells and boundaries).  $N_x$  depends on the choice of boundary conditions, and in general  $N_x \approx 2N_c$ . The spatial grid is numbered from 1 to  $N_x$ , and those with odd index ( $x_1, x_3$ , etc.) denote cell centres, while even-indexed points are cell boundaries. The distribution of spatial grid points is determined by

$$x_1 = 0, \quad x_k = x_{k-1} + \frac{\Delta x_m^c}{2},$$

where  $m = k$  if  $k$  is odd, or  $m = k - 1$  if  $k$  is even.  $\Delta x_m^c$  denotes the cell width of the cell whose centre is at  $m$ . The code supports defining  $\Delta x_m^c$  arbitrarily, but the two most commonly used grids are uniform and “logarithmic”. The second option involves using an exponential function that starts at a prescribed width for the first cell  $dx$ , and drops to a prescribed width of the last cell  $\Delta x_L$ . In this way, the stronger spatial gradients close to the divertor target can be better resolved, while computational power is not wasted in over-resolving the relatively flat upstream.

The choice of a staggered grid avoids the “checkerboard” problem, where odd and even cells

decouple [111]. On the staggered grid variables are placed in the following manner:

- In cell centres:
  - $f_l$  for even  $l$
  - Neutral state densities  $n_b$
  - Ion densities  $n_i$
  - Electron fluid densities  $n_e$
  - Electron fluid temperatures  $T_e$
- On cell boundaries:
  - $f_l$  for odd  $l$
  - $E$ -field
  - Ion velocities  $u_i$
  - Electron fluid velocities  $u_e$

Those variables not evolved in cell centres are simply linearly interpolated from neighbouring cell boundaries, and vice versa. A sketch of a uniform spatial grid used in the standard SOL domain is presented in Figure 4.1. In this case, both the first and the last point on the grid are cell centres, and the point  $x = 0$  and the sheath boundary are included effectively through boundary conditions. Note that due to taking  $x_1 = 0$ , the upstream boundary would be at position  $x = -\Delta x_1^c/2$ , instead of  $x = 0$ . This quirk of labeling does not affect the simulations in any way, and the grid has been relabeled in post-processing for production runs in Chapters 5 and 6 by shifting the entire grid, i.e. setting  $x_1 = \Delta x_1^c/2$ .

All moments of the electron distribution function are calculated numerically using the velocity grid defined above. The finite difference form of the  $n$ -th moment of  $f_l$  is simply given by

$$\langle f_l \rangle_n = 4\pi \sum_{k=1}^{N_v} f_l(v_k) v_k^{2+n} \Delta v_k. \quad (4.1)$$

Using equation (4.1) all of the usual moments can be defined. These are

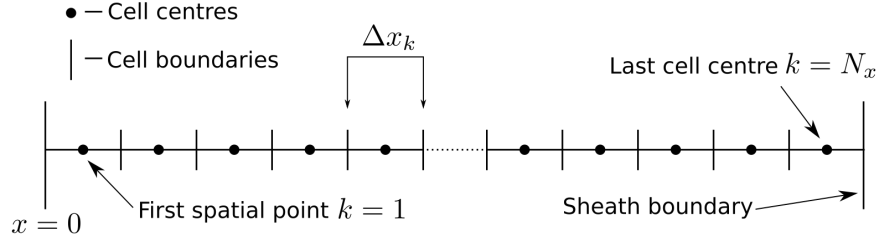


Figure 4.1: An example of a uniform spatial grid for the most widely used SOL domain. Here the upstream and sheath boundary points are not part of the grid.

$$\begin{aligned}
 n_e &= \langle f_0 \rangle_0, \\
 u_e &= \frac{\langle f_1 \rangle_1}{3n_e}, \\
 U_e &= \frac{3}{2} n_e T_e = \langle f_0 \rangle_2 - n_e u_e^2, \\
 j_e &= -en_e u_e, \\
 q_e^{TOT} &= \frac{\langle f_1 \rangle_3}{6}, \\
 P_{11} &= \frac{U_e}{3} + \frac{2}{15} \langle f_2 \rangle_2, \\
 P_{22} = P_{33} &= \frac{\langle f_0 \rangle_2}{3} - \frac{1}{15} \langle f_2 \rangle_2, \\
 q_e &= q_e^{TOT} - u_e \frac{\langle f_0 \rangle_2}{2} - u_e P_{11},
 \end{aligned}$$

### 4.3 Backward Euler method with fixed-point iteration

In order to evolve the time-dependant quantities in the SOL-KiT model, a first-order backward Euler method is used. All variables are evolved implicitly, making SOL-KiT the first arbitrary harmonic fully implicit VFP code. Let  $F$  be the vector containing all the evolved quantities, and  $M(F)$  the evolution matrix. Then the fully implicit backwards Euler method is given by

$$\frac{F^{i+1} - F^i}{\Delta t} = M(F^{i*})F^{i+1}, \quad (4.2)$$

or

$$F^{i+1} = (I - \Delta t M(F^{i*}))^{-1} F^i, \quad (4.3)$$

where  $i^*$  denotes the previous fixed-point iteration, and  $I$  is the identity matrix. Fixed-point iterations are utilised in order to implicitly treat the nonlinear terms in the various equations of the model. For the first iteration in each timestep  $i^* = i$ , and is subsequently updated with  $i + 1$  until convergence of a suitably defined quantity (e.g. the L2 norm of the variable vector) is established within a prescribed tolerance. Implicit variables (those that appear at time  $i + 1$  on RHS of equation (4.2)) in most important nonlinear terms are given in Tables 4.1 - 4.3. Full discretised equations are given in Appendix D, while general spatial and velocity derivatives are covered in the next section. SOL-KiT offers two options for the timestep  $\Delta t$  in (4.2). The

Table 4.1: Fluid continuity and velocity equation implicit variables in nonlinear terms (including fluid contribution to Ampère-Maxwell law)

| Term         | $\frac{\partial(nu)}{\partial x}$ | $S_{ion}^a$ | $S_{rec}^a$ | $-u \frac{\partial F}{\partial x}$ | $\frac{\partial(nkT)}{\partial x}$ | $-\frac{u}{n}S$ | $R_u$ | $R_{en}$       | $\frac{\partial E}{\partial t}$ |
|--------------|-----------------------------------|-------------|-------------|------------------------------------|------------------------------------|-----------------|-------|----------------|---------------------------------|
| Implic. var. | $u$                               | $n_b$       | $n_e^b$     | $F$                                | $n$                                | $u$             | $u$   | $n_b$ or $n_e$ | $u$                             |

<sup>a</sup> Collisional-Radiative model uses the same implicit variable as in sources.

<sup>b</sup> If using kinetic model this is replaced by  $4\pi \int v^2 f_0 dv$ .

Table 4.2: Fluid temperature equation implicit variables in nonlinear terms;  $S$  in fifth term refers to same variable as in  $S_{ion}$  and  $S_{rec}$  of Table 4.1

| Term         | $-u \frac{\partial T}{\partial x}$ | $-T \frac{\partial u}{\partial x}$ | $q_T$ | $q_u$ | $-\frac{S}{n} [\frac{3}{2}kT - u^2]$ | $\frac{u}{n}R_T$ | $\frac{u}{n}R_u$ | $\frac{u}{n}R_{en}$ |
|--------------|------------------------------------|------------------------------------|-------|-------|--------------------------------------|------------------|------------------|---------------------|
| Implic. var. | $T$                                | $u$                                | $T$   | $u$   | $S$                                  | $T$              | $u$              | $n_b$ or $n_e$      |

Table 4.3: Electron kinetic equation implicit variables in nonlinear terms; Coulomb collision terms for  $f_0$  written out in more detail to avoid confusion (see below). Electron-electron collision terms for  $f_{l>0}$  omitted due to complexity (see below and Appendix D.3).

| Term         | $E \frac{\partial f}{\partial v}$ | $\left(\frac{\delta f_0}{\delta t}\right)_{e-e}$             | $\left(\frac{\delta f_{l>0}}{\delta t}\right)_{e-i}^{stationary}$ | $\left(\frac{\delta f_{l>0}}{\delta t}\right)_{e-i}^{moving}$ | $\left(\frac{\delta f_l}{\delta t}\right)_{e-n}$ |
|--------------|-----------------------------------|--------------------------------------------------------------|-------------------------------------------------------------------|---------------------------------------------------------------|--------------------------------------------------|
| Implic. var. | $E$                               | $C^{i*}, D^{i*}, f_0^{i+1}, \partial f_0^{i+1} / \partial v$ | $f_l$                                                             | $f_l, n_i$ in $I(F_l), J(F_l)$                                | $f_l$                                            |

default option is a uniform timestep of prescribed length. However, in longer kinetic simulations, where reaching equilibrium in an efficient manner is the main goal, and temperature and density profiles are prone to some temporal variation, a variable timestep that captures the change in collisionality would be preferred. This is done in the following way. The base timestep is set to a fraction of the normalisation time  $\Delta t = dt_0$ , where usually  $d < 1$ . At each timestep the code rescales  $\Delta t$  to the same fraction of a conservative estimate of the shortest Coulomb collision time  $\Delta t = dt_0 \min(T_e(x)^{3/2} / n_{TOT}(x))$  (where  $n_{TOT}$  is the total density of heavy particles). The choice  $d < 1$  ensures that the shortest collision time is always resolved. In the following text the timestep will be assumed uniform, but generalisation to adaptive timesteps is straightforward.

The structure of the variable vector (with all variables present) is the following:

$$F = \begin{pmatrix} F_{loc}(x_1) \\ F_{loc}(x_2) \\ \vdots \\ F_{loc}(x_{N_x}) \end{pmatrix}, \quad (4.4)$$

where  $F_{loc}(x_k)$  is the (spatially) local subvector for quantities at point  $x_k$  given as

$$F_{loc}(x_k) = \begin{pmatrix} f_{l_{max}}(x_k) \\ f_{l_{max}-1}(x_k) \\ \vdots \\ f_0(x_k) \\ F_n(x_k) \\ E(x_k) \\ F_{fluid}(x_k) \end{pmatrix}, \quad (4.5)$$

where  $l_{max}$  the highest resolved harmonic, and  $f_l(x_k)$  the  $l$ -th harmonics subvector

$$f_l(x_k) = \begin{pmatrix} f_l(x_k, v_1) \\ f_l(x_k, v_2) \\ \vdots \\ f_l(x_k, v_{N_v}) \end{pmatrix}, \quad (4.6)$$

$F_n(x_k)$  contains local neutral state densities (with  $N_n$  being the total number of neutral states tracked)

$$F_n(x_k) = \begin{pmatrix} n_1(x_k) \\ n_2(x_k) \\ \vdots \\ n_{N_n}(x_k) \end{pmatrix}, \quad (4.7)$$

and  $F_{fluid}$  contains local electron and ion fluid quantities

$$F_{fluid}(x_k) = \begin{pmatrix} n_e(x_k) \\ u_e(x_k) \\ T_e(x_k) \\ n_i(x_k) \\ u_i(x_k) \end{pmatrix}. \quad (4.8)$$

Not all variables are always present. The obvious exclusions would be the neutral states when they are not considered, or any harmonics deemed unnecessary. In kinetic mode, the vector does not contain electron fluid quantities, while when fluid electron equations are solved, the distribution function harmonics are not evolved, but are updated after each timestep to be a slowly drifting Maxwellian with current temperature, density, and electron fluid velocity given by

$$f_0(x_k, v_n) = n_e(x_k) (\pi T_e(x_k))^{-3/2} e^{-v_n^2/T_e(x_k)}, \quad (4.9)$$

$$f_1(x_k, v_n) = \frac{2u_e(x_k)v_n}{T_e(x_k)} f_0(x_k, v_n). \quad (4.10)$$

The variable vector length can be calculated easily based on the grid sizes,  $N_x$  and  $N_v$ , as well as the number of harmonics and neutral states,  $l_{max}$  and  $N_n$ . For a kinetic run the length is given by

$$N_{total} = N_x ((l_{max} + 1)N_v + N_n + 3). \quad (4.11)$$

For a representative kinetic system with  $l_{max} = 5$ ,  $N_v = 80$ ,  $N_n = 30$ , and  $N_x = 128$  this gives  $N_{total} = 55424$ . To solve the sparse matrix system that results from such a problem, SOL-KiT uses the MPI and PETSc libraries [112, 113, 114] for both building and solving the matrix system in parallel. The default choice of Krylov subspace method for solving the resulting sparse matrix in SOL-KiT is the biconjugate gradient stabilised method (BiCGSTAB), and the default preconditioner used is the Block Jacobi preconditioner.

## 4.4 General discretisation

The velocity space derivatives appearing in the various kinetic operators are all implemented using a central difference scheme:

$$\begin{aligned} \frac{\partial^2 F}{\partial v^2}(x_k, v_n) &= \frac{1}{\Delta v_n} \left[ \frac{F(x_k, v_{n+1}) - F(x_k, v_n)}{v_{n+1} - v_n} - \frac{F(x_k, v_n) - F(x_k, v_{n-1})}{v_n - v_{n-1}} \right], \\ \frac{\partial F}{\partial v}(x_k, v_n) &= \frac{F(x_k, v_{n+1}) - F(x_k, v_{n-1})}{v_{n+1} - v_{n-1}}, \end{aligned}$$

where  $F$  is any velocity space function. This would, in principle, make the code second order accurate in velocity space. However, the addition of complex collision operators and boundary conditions makes this harder to test.

Spatial derivatives are mostly discretised using an analogous central difference scheme to the above velocity space one. The only exceptions are the advection terms in the momentum and temperature equations (eq. (3.3),(3.7),(3.12)), where an upwind scheme can be used instead of the central difference, reducing those terms to first order accuracy. The upwind scheme used is

simply

$$\frac{\partial F}{\partial t}(x_k) = -u(x_k) \frac{\partial F}{\partial x}(x_k), \quad (4.12)$$

where if  $u(x_k) \geq 0$

$$\frac{\partial F}{\partial x}(x_k) = \frac{F(x_k) - F(x_{k-1})}{x_k - x_{k-1}}, \quad (4.13)$$

and if  $u(x_k) < 0$

$$\frac{\partial F}{\partial x}(x_k) = \frac{F(x_{k+1}) - F(x_k)}{x_{k+1} - x_k}, \quad (4.14)$$

where if  $F$  is not evolved on  $x_{k\pm 1}$  the value at  $x_{k\pm 2}$  is used instead (this is the case for temperature advection in (3.7)). Finally, the diffusion type derivatives are given by

$$\begin{aligned} \frac{\partial}{\partial v} \left( A \frac{\partial F}{\partial v} \right) (x_k, v_n) &= \frac{1}{\Delta v_n} [A(x_k, v_{n+1/2}) \frac{F(x_k, v_{n+1}) - F(x_k, v_n)}{v_{n+1} - v_n} \\ &\quad - A(x_k, v_{n-1/2}) \frac{F(x_k, v_n) - F(x_k, v_{n-1})}{v_n - v_{n-1}}], \\ \frac{\partial}{\partial x} \left( A \frac{\partial F}{\partial x} \right) (x_k) &= \frac{1}{x_{k+2} - x_{k-2}} [A(x_{k+1}) \frac{F(x_{k+2}) - F(x_k)}{x_{k+2} - x_k} \\ &\quad - A(x_{k-1}) \frac{F(x_k) - F(x_{k-2})}{x_k - x_{k-2}}], \end{aligned}$$

where the velocity grid boundaries  $v_{n+1/2}$  are given as  $v_{n+1/2} = \sum_{l=1}^n \Delta v_l$ . The only simple derivatives that do not obey the above are in the velocity advection terms, where in equations (3.25) and (3.26) the conservative form is used

$$\frac{\partial F}{\partial v}(x_k, v_n) = \frac{F(x_k, v_{n+1/2}) - F(x_k, v_{n-1/2})}{\Delta v_n},$$

where  $F(x_k, v_{n+1/2})$  is obtained through linear interpolation. The following velocity space boundary conditions are assumed for the distribution function harmonics

$$f_0(x_k, 0) = \frac{f_0(x_k, v_1) - f_0(x_k, v_2)v_1^2/v_2^2}{1 - v_1^2/v_2^2}, \quad (4.15)$$

$$f_{l>0}(x_k, 0) = 0, \quad (4.16)$$

i.e.  $f_0$  at  $v = 0$  is quadratically extrapolated (this is used whenever  $f_0$  at  $v = 0$  is required) and higher harmonics are set to 0. At the velocity space boundary after  $v_{N_v}$  all  $f_l$  and their derivatives are assumed to be zero.

Finally, it is worth commenting here on how Ampère-Maxwell's law is discretised

$$\left(\frac{\partial E}{\partial t}\right)^{i+1}(x_k) = -A_{EJ}(j_e^{i+1}(x_k) + Zn_i^{i*}(x_k)u_i^{i+1}(x_k)), \quad (4.17)$$

where in kinetic mode the electron current is given by the corresponding moment of  $f_1$ , as defined above, and in the fluid mode it is simply  $j_e^{i+1}(x_k) = n_e^{i*}(x_k)u_e^{i+1}(x_k)$ . The normalisation constant  $A_{EJ} = t_0^2 e^2 n_0 / (\epsilon_0 m_e) = t_0^2 \omega_p^2$  represents the square of the ratio between the plasma oscillation frequency  $\omega_p = \sqrt{e^2 n_0 / (\epsilon_0 m_e)}$  and the reference plasma collision frequency  $1/t_0$ . As this constant tends to be very large, Ampère-Maxwell's law increases the stiffness of the evolution matrix.

## 4.5 Discretisation of Coulomb collision operators

As the core of SOL-KiT is its comprehensive collision operator suite, a brief overview of the Coulomb collision operator discretisation is appropriate. More on the general discretisation can be found in Appendix D.3.

Coulomb collisions treated in the model are both electron-electron and electron-ion collisions. These are further classified based on the distribution function harmonic they act on as either  $l = 0$  operators or  $l > 0$  operators. Electron-electron collisions are included for all harmonics, while electron-ion collisions are included only for  $l > 0$ .

**Electron-electron collisions for  $l = 0$ :** The Chang-Cooper-Langdon[115, 116, 117] method is used for treating electron-electron collisions for the lowest harmonic. The implementation in SOL-KiT is very similar to that in IMPACT[102], and the basic outline of the method is presented here. The collision operator can be written as a divergence of fluxes  $F$

$$\left(\frac{\partial f_0}{\partial t}\right)_{e-e}^{i+1}(x_k, v_n) = \frac{A_{ee}^0 \ln \Lambda_{ee}(T_e^i(x_k), n_e^i(x_k))}{v_n^2} \frac{F^{i+1}(x_k, v_{n+1/2}) - F^{i+1}(x_k, v_{n-1/2})}{\Delta v_n}, \quad (4.18)$$

where  $A_{ee}^0 = \Gamma_{ee}^0 n_0 t_0 / v_{th}^3 = 1 / (Z \ln \Lambda_{ei}(T_0, n_0))$ , and the flux is given by

$$\begin{aligned} F^{i+1}(x_k, v_{n+1/2}) &= C^{i*}(x_k, v_{n+1/2}) f_0^{i+1}(x_k, v_{n+1/2}) \\ &+ D^{i*}(x_k, v_{n+1/2}) \frac{f_0^{i+1}(x_k, v_{n+1}) - f_0^{i+1}(x_k, v_n)}{v_{n+1} - v_n}. \end{aligned} \quad (4.19)$$

$f_0^{i+1}(x_k, v_{n+1/2})$  is then calculated using a special weighted interpolation, which ensures relaxation to a Maxwellian

$$f_0^{i+1}(x_k, v_{n+1/2}) = (1 - \delta^{i*}(x_k, v_{n+1/2}))f_0^{i+1}(x_k, v_{n+1}) + \delta^{i*}(x_k, v_{n+1/2})f_0^{i+1}(x_k, v_n), \quad (4.20)$$

$$\delta^{i*}(x_k, v_{n+1/2}) = \frac{1}{W^{i*}(x_k, v_{n+1/2})} - \frac{1}{\exp[W^{i*}(x_k, v_{n+1/2})] - 1}, \quad (4.21)$$

$$W^{i*}(x_k, v_{n+1/2}) = (v_{n+1} - v_n) \frac{C^{i*}(x_k, v_{n+1/2})}{D^{i*}(x_k, v_{n+1/2})}. \quad (4.22)$$

The friction coefficient is

$$C^{i*}(x_k, v_{n+1/2}) = 4\pi \sum_{l=1}^n f_0^{i*}(x_k, v_l) v_l^2 \Delta v_l. \quad (4.23)$$

As previously noted in Section 3.4.2, the diffusion coefficient  $D$  is written in a way that is different from the standard form in the literature. This allows discretisation[117] that conserves electron energy as well

$$D^{i*}(x_k, v_{n+1/2}) = \frac{4\pi}{v_{n+1/2}^*} \sum_{l=1}^n v_l^2 \left[ \sum_{m=l}^{N_v-1} f_0^{i*}(x_k, v_{m+1/2}) v_{m+1/2} (v_{m+1} - v_m) \right] \Delta v_l, \quad (4.24)$$

where  $v_{n+1/2}^* = (v_n + v_{n+1})/2$ . Boundary conditions for the  $C$  and  $D$  coefficients are taken in such a way to conserve particle density (see [102, 116]). The resulting submatrix from this operator is tridiagonal. Using an iterative method both particles and energy are conserved up to nonlinear iteration tolerance. Furthermore, the electron distribution function collisionally relaxes to a Maxwellian in the absence of other driving forces.

**Electron-electron collisions for  $l > 0$ :** Electron-electron collision terms for higher  $l$  (equation (3.34)) are normalised in the same way as the  $l = 0$  term, and are discretised following a method similar to that used in the code OSHUN [101]. Basic elements of this discretisation are presented here. The first three terms in (3.34) produce a tridiagonal matrix when discretised. Remaining terms produce an upper and lower triangular submatrix due to the  $I$  and  $J$  integrals, which are discretised as

$$I_j[f_l](x_k, v_n) = 4\pi \begin{pmatrix} \left(\frac{v_1}{v_n}\right)^j v_1^2 \Delta v_1 \\ \left(\frac{v_2}{v_n}\right)^j v_2^2 \Delta v_2 \\ \vdots \\ \left(\frac{v_{n-1}}{v_n}\right)^j v_{n-1}^2 \Delta v_{n-1} \\ \frac{1}{2} v_n^2 \Delta v_n \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T \cdot \begin{pmatrix} f_l(x_k, v_1) \\ \vdots \\ f_l(x_k, v_N) \end{pmatrix}, \quad (4.25)$$

$$J_j[f_l](x_k, v_n) = 4\pi \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \frac{1}{2} v_n^2 \Delta v_n \\ \left(\frac{v_{n+1}}{v_n}\right)^j v_{n+1}^2 \Delta v_{n+1} \\ \vdots \\ \left(\frac{v_{N_v-1}}{v_n}\right)^j v_{N_v-1}^2 \Delta v_{N_v-1} \\ \left(\frac{v_{N_v}}{v_n}\right)^j v_{N_v}^2 \Delta v_{N_v} \end{pmatrix}^T \cdot \begin{pmatrix} f_l(x_k, v_1) \\ \vdots \\ f_l(x_k, v_N) \end{pmatrix}. \quad (4.26)$$

For  $l = 1$  the discretised electron-electron collision operator does not numerically conserve momentum. This is due to it not being written in a form that is exclusively diffusive. However, the numerically lost momentum is transferred to the ions by the code algorithm, and total momentum is thus conserved.

**Electron-ion collisions:** The electron-ion operator for stationary cold ions is trivial, and is discretised straightforwardly. The moving ion operator is discretised similarly to the electron-electron operator for higher  $l$ , with the exception of having mainly a tridiagonal component, and a part where ion density is the implicit variable (if working on a cell boundary, it is implicitly interpolated). For the second part the previously presented  $I(F_l)$  and  $J(F_l)$  integrals for cold ions ((3.38) and (3.39)) are required. For a given lagged (evaluated at  $i^*$ ) ion velocity  $u_i^{i^*}(x_k)$

and density  $n_i^{i+1}(x_k)$  these integrals in discrete form are

$$I_j^{i+1}[F_l](x_k, v_n) = (2l + 1)n_i^{i+1}(x_k) \frac{u_i^{i*}(x_k)^j}{v_n^j} \Theta(v_k - u_i^{i*}(x_k)), \quad (4.27)$$

$$J_j^{i+1}[F_l](x_k, v_n) = (2l + 1)n_i^{i+1}(x_k) \frac{u_i^{i*}(x_k)^j}{v_n^j} \Theta(u_i^{i*}(x_k) - v_k). \quad (4.28)$$

In the same vein as the electron-electron operator above, the electron-ion operator for  $l = 1$  suffers from numerically lost momentum, and this will be addressed in the benchmarking section below.

All operators discussed in this section are presented in their full form in Appendix D.

## 4.6 Electron-neutral collision numerics

Electron-neutral collisions implemented in SOL-KiT are both elastic collisions, as well as inelastic collisions associated with the various electron-hydrogen reactions. In this work, inelastic electron-hydrogen collision operators are the only one used, and their conservative discretisation will be the main topic of this section. However, the basic properties of the elastic electron-neutral collision operator will be presented before focusing on the conservative discretisation.

**Elastic collisions:** The discretisation of elastic collisions borrows greatly from the Coulomb collision operators. Equation (3.42) is discretised in a way similar to the Chang-Cooper-Langdon scheme. However, since the integral is linear in  $f_0$ , there is no need for special interpolation ( $f_0$  and  $\sigma$  are simply linearly interpolated), and just the flux formalism was used, with the  $C$  and  $D$  coefficients (here left un-normalised) being

$$C(v_{n+1/2}) = n_b v_{n+1/2}^4 \sigma^{el}(v_{n+1/2}), \quad (4.29)$$

$$D(v_{n+1/2}) = n_b v_{n+1/2}^3 \sigma^{el}(v_{n+1/2}) \frac{kT_g}{m_e}, \quad (4.30)$$

where

$$\sigma^{el}(v_n) = \int d\Omega (1 - \cos \chi) \sigma^{el}(\chi, v_n). \quad (4.31)$$

For the constant cross-section (3.44), this is simply equal to it.

The above discretisation produces an operator that conserves particle number and relaxes the electron  $f_0$  to a Maxwellian with temperature  $T_g$  (within finite grid effects). For higher  $l$ , equation (3.43) is discretised in a straightforward way

$$\left( \frac{\partial f_l}{\partial t} \right)_{b, el-en}^{i+1}(x_k, v_n) = -n_b(x_k) v_n \sigma_{el,b}^1(v_n) f_l^{i+1}(x_k, v_n). \quad (4.32)$$

#### 4.6.1 Conservative discretisation scheme for inelastic collisions

In order to streamline the arguments in the upcoming sections, it is beneficial to introduce the following notation. If inelastic processes with transition energy  $\epsilon$  are labeled as  $\Pi$ , the corresponding superelastic (inverse) processes (with transition energy  $-\epsilon$ ) can be labeled as  $\Pi^{-1}$ . Furthermore, since energy and particle conservation is governed by the  $l = 0$  harmonic, it will be denoted simply as  $f$  in the following derivation. Then the value of  $f$  in the  $n$ -th velocity cell centre can be written as  $f_n$ , while the total cross-section at the same point is  $\sigma_n$ .

Equation (3.46) contains two terms, a loss/emission term and a gain/absorption term. The conservative discretisation problem stems from the fact that, while the emission term is defined on the used velocity grid, the absorption term requires evaluation of the distribution function on (most likely) non-existent points  $\alpha(v)v$  (where  $\alpha = (1 \pm 2\epsilon/mv^2)^{1/2}$ ). Straightforward interpolation of  $f$  and  $\sigma$  here fails to produce a conservative discretisation. This and the following two sections are devoted to the development of such a conservative scheme.

The first step is to write the collision operator in the emission/absorption form

$$C_n = -E_n + A_n, \quad (4.33)$$

where

$$E_n = n_{neut} v_n f_n \sigma_n, \quad (4.34)$$

and

$$A_n = \sum_m W_{nm} E_m, \quad (4.35)$$

where  $W_{nm}$  are weights determining the contribution of the emission from cell  $m$  to the absorption in cell  $n$ . These weights are determined by the process ( $\Pi$  or  $\Pi^{-1}$ ) and the velocity grid, and will be tuned to ensure conservation. Note that all quantities here are normalised, with the normalisation constant dropped for simplicity of notation. The next step is to translate conservation constraints into constraints onto  $W_{nm}$ .

For particle conservation, the number of particles emitted by a single cell  $m$  -  $4\pi E_m v_m^2 \Delta v_m$  must be absorbed exactly by some other cells  $n$  -  $4\pi A_n v_n^2 \Delta v_n$

$$4\pi E_m v_m^2 \Delta v_m = 4\pi \sum_n W_{nm} E_m v_n^2 \Delta v_n, \quad (4.36)$$

which yields the following particle conservation condition

$$v_m^2 \Delta v_m = \sum_n W_{nm} v_n^2 \Delta v_n. \quad (4.37)$$

For energy conservation, all energy being emitted via collisions from any single cell needs to either be lost to the energy of internal atomic states or be absorbed by some other cells  $n$ . The energy lost to atomic states by electrons in cell  $m$  is simply  $\pm 4\pi \epsilon E_m v_m^2 \Delta v_m$ , where the sign denotes whether the process is inelastic or superelastic. Thus, energy balance for an emitting cell  $m$  is

$$4\pi E_m v_m^4 \Delta v_m = 4\pi \sum_n W_{nm} E_m v_n^4 \Delta v_n \pm 4\pi \epsilon E_m v_m^2 \Delta v_m, \quad (4.38)$$

from which the energy conservation condition is obtained

$$v_m^2 \Delta v_m (v_m^2 \mp \epsilon) = \sum_n W_{nm} v_n^4 \Delta v_n. \quad (4.39)$$

The final important condition to be written in discretised form is the detailed balance condition for collisional cross-sections of inverse processes. As an example, the result for

deexcitation ( $\Pi = ex$ ,  $\Pi^{-1} = deex$ ) is presented here, with the same procedure applicable to recombination. In essence, detailed balance is the state where for a Maxwellian distribution of electrons and for a Boltzmann distribution of excited states the rates of excitation and deexcitation become equal. This can be written as

$$n_l \sum_m f_m \sigma_m^{ex} v_m^3 \Delta v_m = n_u \sum_n f_n \sigma_n^{deex} v_n^3 \Delta v_n, \quad (4.40)$$

where  $n_l$  and  $n_u$  denote the densities of the lower and upper excited states, respectively. Using a Maxwellian  $f_m \propto \exp(-v_m^2/T)$  and relating  $n_u$  and  $n_l$  via the Boltzmann distribution  $n_u = n_l g_u / g_l \exp(-\epsilon/T)$ , the numerical detailed balance condition is

$$\sigma_n^{deex} = \frac{g_l}{g_u} e^{\epsilon/T} \sum_m W_{nm} \sigma_m^{ex} \frac{v_m}{v_n} e^{-(v_m^2 - v_n^2)/T}, \quad (4.41)$$

where (4.37) was used to eliminate the sum over  $n$ . Note the dependence on temperature and the excitation weights. This is due to the discrete nature of the grid, where energy differences between absorbing and emitting cells do not have to be equal to the analytical value  $\epsilon$ . It is, however, easy to see that for a perfectly analytical grid where  $\epsilon = v^m - v^n$  and  $W_{nm} = v_n / v_m \delta_{nm}$  (see below) the expression reduces to the straightforward discretisation of (3.50).

### 4.6.2 Two-absorber mapping

In the above conservation conditions the summation range for  $n$  was left unspecified. The simplest way to determine this is the following. For each emitter cell  $m$  two consecutive absorber cells,  $n_1$  and  $n_2$ , are chosen, such that  $\sqrt{v_m^2 \mp \epsilon}$  lies between  $v_{n_1}$  and  $v_{n_2}$ . These two points will be referred to as the ideal absorber pair. In this way, no further instructions on partitioning the emitted particles and energy are necessary, and the weights  $W_{nm}$  can be calculated. Since for any given  $m$  there are only two absorbing cells, these can be denoted simply as  $W_1^m$  and  $W_2^m$ , and solving the two conservation conditions yields

$$W_1^m = \frac{v_m^2 \Delta v_m}{v_{n_1(m)}^2 \Delta v_{n_1(m)}} \left( 1 - \frac{v_m^2 - v_{n_1(m)}^2 \mp \epsilon}{v_{n_2(m)}^2 - v_{n_1(m)}^2} \right), \quad (4.42)$$

$$W_2^m = \frac{v_m^2 \Delta v_m}{v_{n_2(m)}^2 \Delta v_{n_2(m)}} \frac{v_m^2 - v_{n_1(m)}^2 \mp \epsilon}{v_{n_2(m)}^2 - v_{n_1(m)}^2}. \quad (4.43)$$

Figure 4.2 shows an illustration of this mapping for an excitation collision with both particle and energy transfer obeying conservation conditions.

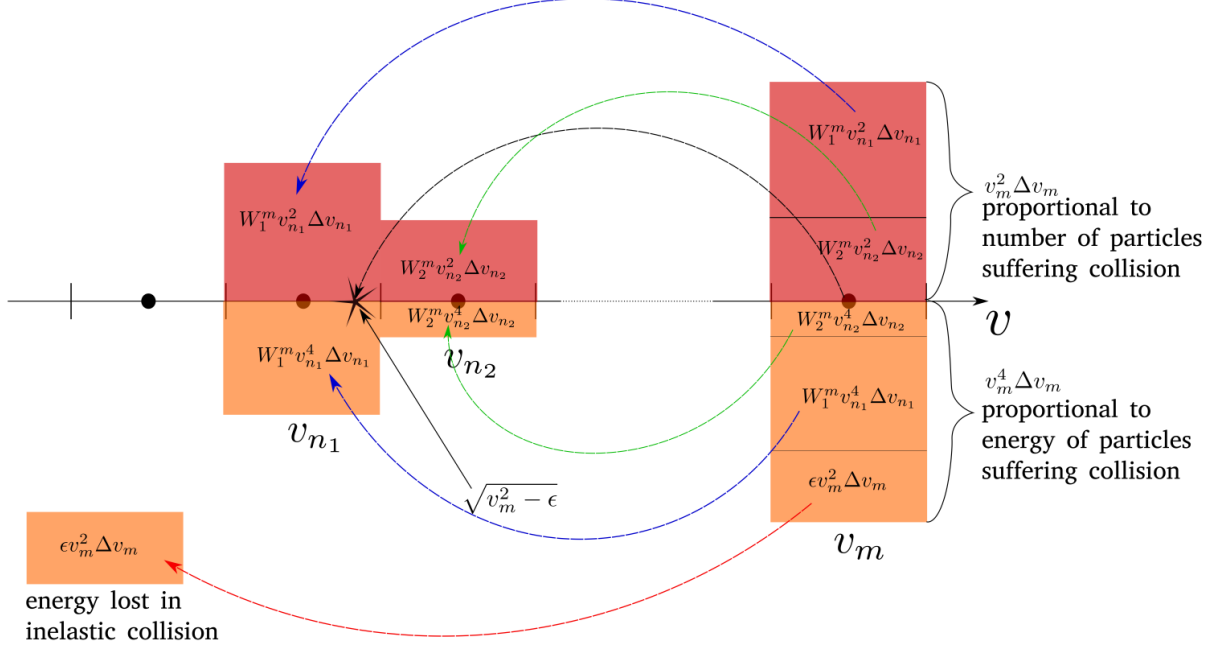


Figure 4.2: Two-absorber mapping for an excitation collision; particles and energy emitted by the higher energy cell is distributed among the two absorbers, while a portion of energy is lost to internal energy states of the collision target (atom) - red line. Blue and green lines denote emission to first and second cell of absorber pair, respectively. The black star shows the location of the analytical absorption point.

To establish that this scheme can reduce to the analytical result, two properties expected in the analytic limit must be noted. Firstly,  $n_1 \rightarrow n_2 = n$ , i.e. each emitting point has one and only one absorbing point. To enforce this, one can simply let one of the weights tend to 0. For the sake of this illustrative argument, let that be  $W_1^m$ . An equivalent result would be obtained if  $W_2^m$  was chosen. From  $W_1^m \rightarrow 0$  it is easily surmised that  $W_2^m \rightarrow \alpha(v_n)^2 \Delta v_m / \Delta v_n$  (since  $v_m = \alpha(v_n) v_n$  in the analytical limit). Taking the differential of (3.45) points towards a grid that satisfies

$$\Delta v_m / \Delta v_n \rightarrow 1 / \alpha(v_n)$$

which finally yields the limits

$$W_1^m \rightarrow 0, \quad W_2^m \rightarrow \alpha(v_n).$$

The gain term  $A$  then becomes

$$A_n = \alpha(v_n)E_m,$$

which, upon expanding the emission term, is

$$A_n = n_{neut}\alpha(v_n)v_m f_m \sigma_m.$$

Remembering again that  $v_m = \alpha(v_n)v_n$  the analytical limit of the gain term is finally written as

$$A_n = n_{neut}\alpha(v_n)^2 v_n f_m \sigma_m,$$

which is equivalent to the second term in equation (3.46), and thus the analytical  $\alpha^2$  form is recovered.

At first glance, the two-absorber mapping appears adequate, as it conserves both particles and energy, but after a closer look at (4.41) a potential problem reveals itself. Consider the pathological case in an excitation process  $W_{nm} = 0$  for some  $n$  and every  $m$ . In this case  $\sigma_n^{deex} = 0$  for the corresponding deexcitation process. This implies that if cell  $n$  does not absorb in process  $\Pi$ , it will not emit in  $\Pi^{-1}$ , producing gaps in the velocity grid where cells that should emit do not. This is not physical, and the mapping needs to be refined.

### 4.6.3 Two-absorber mapping with pair partition

In the previous section every emitter cell  $m$  was associated with an ideal absorber pair  $(n_1(m), n_2(m))$ . For the following discussion it becomes necessary to define the absorber list of point  $m$ ,  $\mathcal{A}_m^\Pi$ , in process  $\Pi$ , which contains all absorber pairs associated with cell  $m$  in process  $\Pi$ . The two-absorber mapping implies  $\mathcal{A}_m^\Pi = \{(n_1(m), n_2(m))\}$ , where the only pair is the ideal absorber pair. As noted above, this produces gaps in the velocity grid where cells do not emit in the inverse process  $\Pi^{-1}$ .

In order to fill out the aforementioned gaps, it is potentially necessary to include absorbers outside the ideal pair. This can be done by scanning over all cells  $n$  that are not in the ideal absorber pair of emitter  $m$ , but whose  $\sqrt{v_n^2 \pm \epsilon}$  (note the change in sign!) falls into cell  $m$ . Cell  $m$  can then be referred to as the ideal emitter of cells  $n$ .

The next step in adapting the two-absorber mapping discussed previously is generating absorber pairs that would include the non-ideal absorbers  $n$ , while satisfying the original constraint, namely that  $\sqrt{v_m^2 \mp \epsilon}$  is between the points of each new pair. In SOL-KiT this is done by always pairing non-ideal absorbers with one of the ideal absorbers. If  $P_m \geq 1$  is the number of (both ideal and non-ideal) absorber pairs of cell  $m$ , the absorber list becomes  $\mathcal{A}_m^\Pi = \{(n_1^p(m), n_2^p(m)), p = 1, \dots, P_m\}$ , where the first and second cell in pair  $p$  are  $n_1^p(m)$  and  $n_2^p(m)$ , respectively.

Now that multiple absorber pairs exist for some of the emitters, a way to partition the emitted energy/particles among pairs is needed. In SOL-KiT, the following simple approach is taken. The first step is defining the total energy width of the entire absorber list and normalising the energy widths of each cell within the list to that total width:

$$\beta_{TOT}^m = \sum_{n \in \mathcal{A}_m^\Pi} 2v_n \Delta v_n, \quad \beta_n = 2v_n \Delta v_n / \beta_{TOT}^m.$$

Defining  $\delta_n$  as the number of pairs in  $\mathcal{A}_m^\Pi$  which contain point  $n$ , one can then define

$$\gamma^p = \frac{\beta_{n_1^p}}{\delta_{n_1^p}} + \frac{\beta_{n_2^p}}{\delta_{n_2^p}} \quad (4.44)$$

to be the fraction of the emission given to pair  $p$ . It can then be shown that  $\sum_{p=1}^{P_m} \gamma^p = 1$ , as one would expect. An example with an absorber list with three distinct cells is given in Figure 4.3.

It is now possible to apply the same method as the one for the two-absorber case, except the final results for  $W_1^m$  and  $W_2^m$  will now be functions of the pair  $p$  for which they have been calculated, and will have an extra  $\gamma^p$  factor multiplying the previous simple results (see below). To then calculate the total absorption term for a given cell  $n$ , it should be summed over each pair the cell belongs to, i.e.

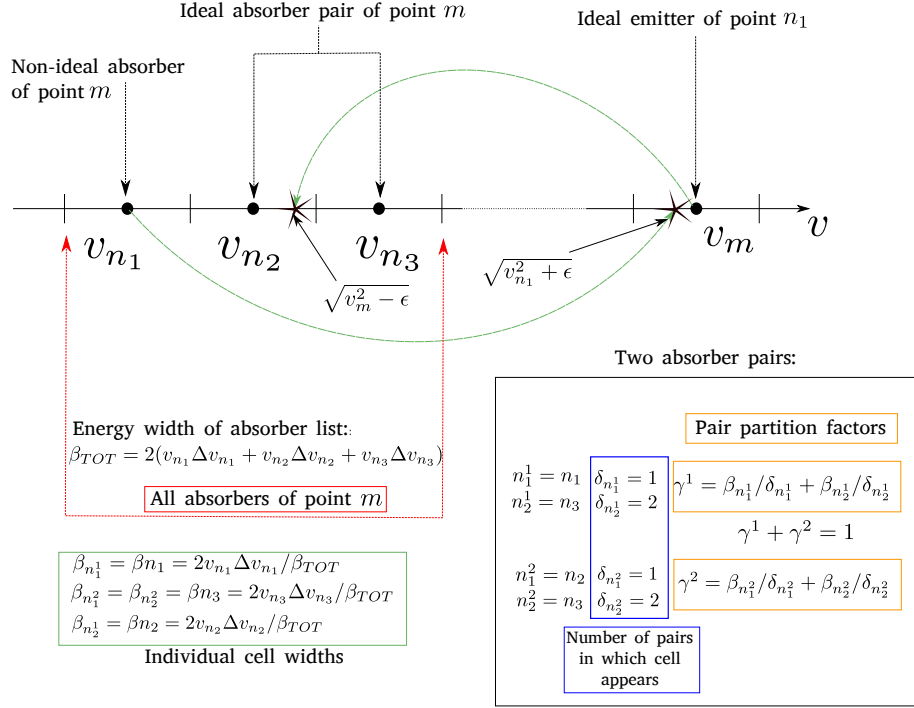


Figure 4.3: Pair partition calculation example for an excitation collision; emitter cell has a list of three absorbers, grouped into two pairs, with emitted energy and particles partitioned according to factors  $\gamma^1$  and  $\gamma^2$

$$A_n = \sum_m \sum_p W_{nm}^p E_m. \quad (4.45)$$

This way both particle and energy conservation have been ensured, and a reasonably physical numerical detailed balance condition has been imposed. The weights in this case are given by

$$W_{n_1^p(m)m} = \gamma_m^p \frac{v_m^2 \Delta v_m}{v_{n_1^p(m)}^2 \Delta v_{n_1^p(m)}} \left( 1 - \frac{v_m^2 - v_{n_1^p(m)}^2 \mp \epsilon}{v_{n_2^p(m)}^2 - v_{n_1^p(m)}^2} \right), \quad (4.46)$$

$$W_{n_2^p(m)m} = \gamma_m^p \frac{v_m^2 \Delta v_m}{v_{n_2^p(m)}^2 \Delta v_{n_2^p(m)}} \frac{v_m^2 - v_{n_1^p(m)}^2 \mp \epsilon}{v_{n_2^p(m)}^2 - v_{n_1^p(m)}^2}, \quad (4.47)$$

with the general weight  $W_{nm}^p$  being then

$$W_{nm}^p = W_{n_1^p(m)m} \delta_{nn_1(m)} + W_{n_2^p(m)m} \delta_{nn_2(m)}, \quad (4.48)$$

where  $\delta$  now indicates Kronecker's delta.

Using the above method for every process produces both a transition mapping and weights for each one. These depend solely on the grid and the inelastic processes being considered, and as such do not change during a simulation. The final discretised (un-normalised) form of the inelastic collision integral for particle conserving collisions is then

$$\begin{aligned} \left( \frac{\delta f_l}{\delta t} \right)_{b \rightarrow b'}^{inel, i+1}(x_k, v_n) = & -n_b^{i*}(x_k) [v_n \sigma_{b \rightarrow b'}^{TOT}(v_n) f_l^{i+1}(x_k, v_n) \\ & - \sum_m \sum_p W_{nm}^p v_m \sigma_{b \rightarrow b'}^{TOT}(v_m) - \sigma_{b \rightarrow b'}^{(l)}(v_m)] f_l^{i+1}(x_k, v_m). \end{aligned} \quad (4.49)$$

## 4.7 Boundary condition numerics

In order to implement the boundary condition at the divertor target, as was implied in Section 3.5, knowledge of the forward going electron distribution function is required. In SOL-KiT it is reconstructed by extrapolating harmonics from cells leading up to the boundary

$$f_{\text{odd } l}^{\text{forward, target}} = \frac{n_e^2(x_{N_x})}{n_e^2(x_{N_x-1})} f_{\text{odd } l}(x_{N_x-1}), \quad f_{\text{even } l}^{\text{forward, target}} = \frac{n_e(x_{N_x})}{n_e(x_{N_x-1})} f_{\text{even } l}(x_{N_x}), \quad (4.50)$$

where the harmonics are scaled by the ratio of the electron densities at spatial cells  $N_x$  and  $N_x - 1$ . The choice to perform this sort of extrapolation, and not a linear one, comes from the danger of large density gradients (which are often present at the divertor target) to produce negative extrapolated densities when extrapolated linearly.

Knowing the forward going distribution allows calculation of the cut-off distribution using equation (3.59), while equation (3.68) imposes  $v_c$ . However, due to the discretisation of velocity space, this will not be one of the resolved cell centres, and interpolation is required in order to calculate the precise cut-off. A diagram of the interpolation region is given in Figure 4.4.

The interpolation replaces cell  $K$  containing the cut-off and its preceding cell  $K - 1$  with two new cells with centres

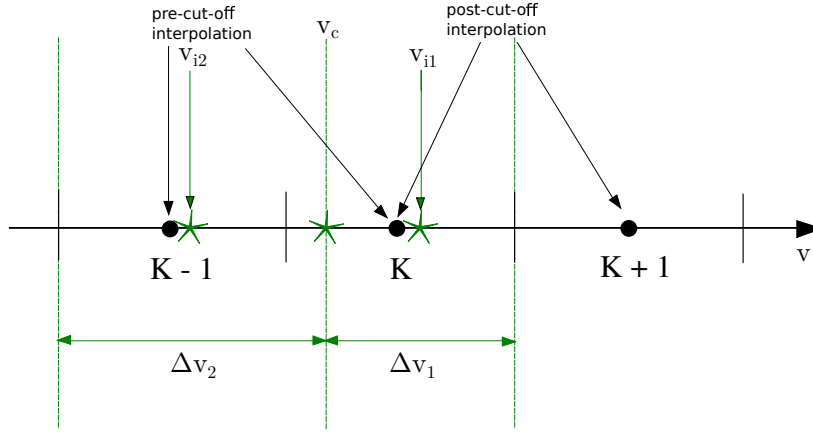


Figure 4.4: The interpolation region on the velocity grid; cell  $K$  contains the cut-off, and cells  $K$  and  $K - 1$  are replaced with interpolated cells with centres at  $v_{i1}, v_{i2}$  and widths  $\Delta v_1, \Delta v_2$

$$v_{i1} = \frac{v_{K+1/2} + v_c}{2}, \quad v_{i2} = \frac{v_{K-3/2} + v_c}{2},$$

and with widths

$$\Delta v_1 = v_{K+1/2} - v_c, \quad \Delta v_2 = v_c - v_{K-3/2}.$$

The electron flux to the boundary (given in equation (3.68)) is then calculated using this updated grid, while linearly interpolating the  $f_1$  component of the cut-off distribution in the two new cells. The electron flux can then be matched to the ion flux using a false position method to find  $v_c$  with a desired accuracy, and the resulting cut-off distribution can be used as an advective boundary condition. In this case, the false position method is used in the following way:

1. The first guess for the cut-off velocity is the value at the first velocity cell boundary that produces an electron flux greater than the ion flux  $\Gamma_i$  - this will always be the left/lower cell boundary of cell  $K$  defined above
2. The first bracketing interval  $(v_a, v_b)$  is now defined as  $(v_{K-1/2}, v_{K+1/2})$
3. The electron flux is calculated at both interval endpoints -  $\Gamma_a, \Gamma_b$
4. To obtain the next cut-off velocity guess the v-intercept of  $\Gamma - \Gamma_i$  is calculated

$$v_c = \frac{v_a(\Gamma_b - \Gamma_i) - v_b(\Gamma_a - \Gamma_i)}{\Gamma_b - \Gamma_a}$$

5. The electron flux is calculated using the new guess  $v_c$  and compared to the ion flux
6. If the desired accuracy has not yet been reached, the new bracketing interval is defined by replacing  $v_a$  with  $v_c$  if the newly calculated electron flux is greater than the ion flux, or  $v_b$  with  $v_c$  if the flux is smaller than the ion flux - go to step 3

## 4.8 Benchmarking of SOL-KiT

An important step in any scientific computing development project is the thorough testing of the produced software package. SOL-KiT in particular has a number of novel numerical and algorithmic aspects that require verification. The remaining sections of this chapter are therefore dedicated to testing properties of the various operators implemented in SOL-KiT. An overview of the performed tests and their scope in terms of targeted operators is given in Table 4.4. In all of the tests the plasma is hydrogenic, i.e.  $Z = 1$ .

Table 4.4: List of performed test runs and sets of runs with their target operators.

| Run/Set  | Targeted operators                                                         |
|----------|----------------------------------------------------------------------------|
| Runs 1-4 | e-i and e-e collisions, Vlasov, Maxwell                                    |
| Runs 5-6 | fluid ion and electron operators                                           |
| Set 1    | e-i and e-e collisions, Vlasov, Maxwell, high $l$                          |
| Runs 7-8 | kinetic e-n inel. collisions, CRM                                          |
| Run 9    | fluid e-n inel. collisions, CRM, detailed balance                          |
| Run 10   | e-i and e-e collisions, Vlasov, Maxwell, kinetic e-n inel. collisions, CRM |
| Run 11   | fluid ion operators - advection                                            |
| Set 2    | fluid ion operators - charge-exchange friction                             |
| Set 3    | fluid ion operators - momentum loss in electron-ion collisions             |
| Set 4    | divertor boundary condition - analytic limit                               |
| Set 5    | divertor boundary condition, high $l$                                      |

### 4.8.1 Heat conduction tests

One of the standard quantities used to test both the collisional and collisionless operators in a VFP code is the heat conductivity. This has been tested in both the local, Spitzer-Härm limit, as well as in a set of non-local simulations.

**Local heat conduction tests** Two types of tests were used to verify the local limit of heat conduction in SOL-KiT. The first type is a small perturbation test[118, 119] on a periodic grid, with the initial temperature given by

$$T(x) = T_0 + T_1 \sin\left(2\pi \frac{x}{L}\right), \quad (4.51)$$

where  $L$  is the total length of the system, given by  $L = N_c \Delta x$ . The density was set to  $n_0 = 10^{19} m^{-3}$ , and the rest of the simulation parameters are

$$T_0 = 100\text{eV}, \quad T_1 = 0.05\text{eV},$$

$$N_c = 64, \quad \Delta x = 150 x_0, \quad N_v = 120,$$

with  $\Delta v, \Delta t$ , and the total number of timesteps being able to vary between runs. The total time simulated was always set to  $30 t_0$ , i.e. to 30 electron-ion collision times. In all runs the full set of Coulomb collision operators was active, and the highest harmonic number was kept at  $l_{max} = 1$ . The calculated conduction heat flux was compared to the Spitzer-Härm (SH) heat flux  $q_{SH}$  (equation (3.8)), with the heat conductivity for  $Z = 1$  in SOL-KiT normalised units being  $\kappa = 0.6\sqrt{\pi}$ .

The ratio of the calculated heat flux and the reference SH flux at the end of each run would be averaged along the simulation domain, and these are the results presented below. Three pure kinetic runs (with initial  $f_1$  set to 0, and no fluid ion operators active) were performed. The reference run (Run 1) with  $\Delta t = 0.1 t_0$ ,  $\Delta v = 0.1 v_{th}$ ,  $N_t = 300$  produces an average heat flux of  $q = (0.988296 \pm 1 \times 10^{-6})q_{SH}$ , i.e. reproduces the reference results with less than 1.2% error. Run 2 used a smaller timestep  $\Delta t = 0.05 t_0$ ,  $N_t = 600$ , but the ratio obtained was the same as in Run 1. Run 3, on the other hand, tested the velocity resolution dependence by setting  $\Delta v = 0.05 v_{th}$ , and the obtained heat flux was  $q = (0.997488 \pm 1 \times 10^{-6})q_{SH}$ , reducing the relative error below 0.3%. At this point the relative error is smaller than the assumed precision of the reference SH flux value, and should thus be taken with a grain of salt.

The next set of small perturbation tests aimed to compare the results of kinetic simulations to those performed using the fluid mode of SOL-KiT. For this purpose, since the fluid model

assumes the reference SH heat flux described above from the very start of the simulation, in the kinetic simulation (Run 4)  $f_1$  was initialised to a local solution which would give the same heat flux as the one in the fluid run (Run 5). Other than this, the parameters of Run 4 were identical to those of Run 1, and the final heat flux ratio was the same as the one there. Run 5 was performed with the same parameters as Run 4, but instead of solving the kinetic equation for the electrons, fluid equations for both electrons and ions were solved. The total changes in the temperature value at its maximum for both runs were compared. It was found that the relative difference in the changes was less than 0.3%, showing good agreement between the kinetic and fluid model in the small perturbation test.

The final heat conduction test run (Run 6) was done for the fluid model, where the plasma was initialised on a logarithmic spatial grid ( $\Delta x = 8.5 x_0$  and  $\Delta x_L = 0.5 x_0$ ) with the Two-Point Model[12] profile

$$T(x) = \left( T_u^{7/2} + \frac{x}{L} (T_u^{7/2} - T_d^{7/2}) \right)^{2/7}, \quad n(x) = n_u T_u / T(x),$$

where  $n_u = 0.368 \times 10^{19} m^{-3}$  and  $T_u = 18\text{eV}$  are the upstream density and temperature, while  $T_d = 5\text{eV}$  is the downstream temperature. Boundary conditions were fixed. It is to be expected that this profile should not evolve, and after 30000 collision times (for a reference plasma of  $n_0 = 2.5 \times 10^{19} m^{-3}$  and  $T_0 = 10\text{eV}$ ), the largest deviation from the initial profile was 0.12 %, which is due to linear interpolation close to the downstream boundary, with most points having less than 0.01% deviation.

**Non-local heat conduction tests** In order to test how SOL-KiT handles a more non-local regime, a set of runs (Set 1) was performed with a setup similar to Run 1 and related runs, featuring a sinusoidal temperature perturbation. For completeness, the common run parameters for Set 1 are

$$T_0 = 100\text{eV}, \quad T_1 = 0.1\text{eV}, \quad n_0 = 10^{19} m^{-3},$$

$$N_c = 63, \quad N_v = 120, \quad \Delta v_1 = 0.0307, \quad c_v = 1.01.$$

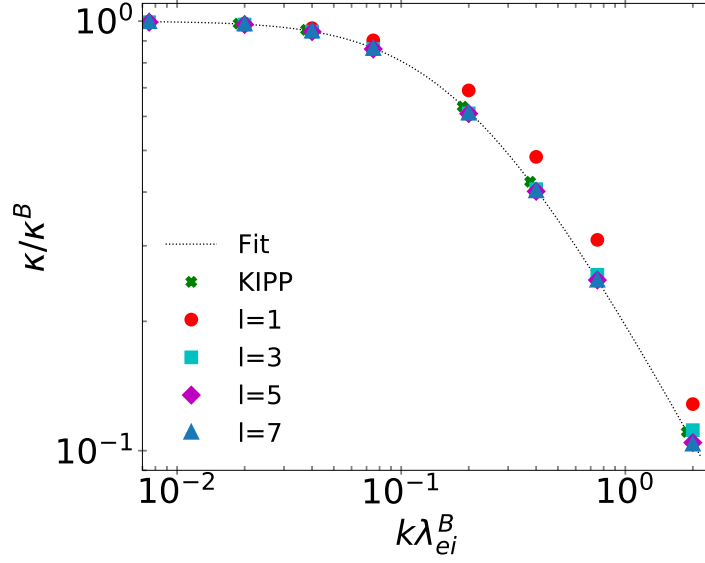


Figure 4.5: Comparison of SOL-KiT and KIPP results into the non-local regime for different number of resolved harmonics. KIPP results have been fitted using equation 4.52. Graph and data analysis courtesy of Abetharan Antony.

The various runs in the set were performed with different system lengths and with varying number of resolved harmonics  $l_{max} = 1, 3, 5, 7$ . In Figure 4.5  $\kappa/\kappa^{(B)} = q/q_{SH}$  is plotted for each of the runs, comparing it with values obtained with the code KIPP[68, 5, 87] and reported by Brodrick et al.[119]. The ratio  $q/q_{SH}$  was obtained by running each run in the set until the ratio equilibrated. The different values in Figure 4.5 are plotted as a function of  $k\lambda_{ei}^{(B)}$ , where  $\lambda_{ei}^{(B)} = 3(\pi/2)^{1/2}x_0/4$  is the Braginskii electron-ion collisional mean freepath, as used by Brodrick et al., and  $k = 2\pi/L$  is the perturbation wavenumber. KIPP results were fitted using the following function based on equation (25) in [119]

$$\frac{\kappa}{\kappa^{(B)}} = \left[ 1 + \left( \frac{1}{a(k\lambda_{ei}^{(B)})^2} + \frac{1}{bk\lambda_{ei}^{(B)}} \right)^{-1} \right]^{-1}, \quad (4.52)$$

where the values obtained for the parameters  $a$  and  $b$  are 51.409789 and 4.4682314, respectively. The increase in number of harmonics leads to an increase in agreement between SOL-KiT and KIPP. Already at  $l = 5$  SOL-KiT results appear to be very close to the fit values, with the increase to  $l = 7$  having a negligible effect on the result. Note also that the diffusive approximation ( $l = 1$ ) appears to break down around  $k\lambda_{ei}^{(B)} = 0.075$ , while the  $l = 3$  approximation seems to

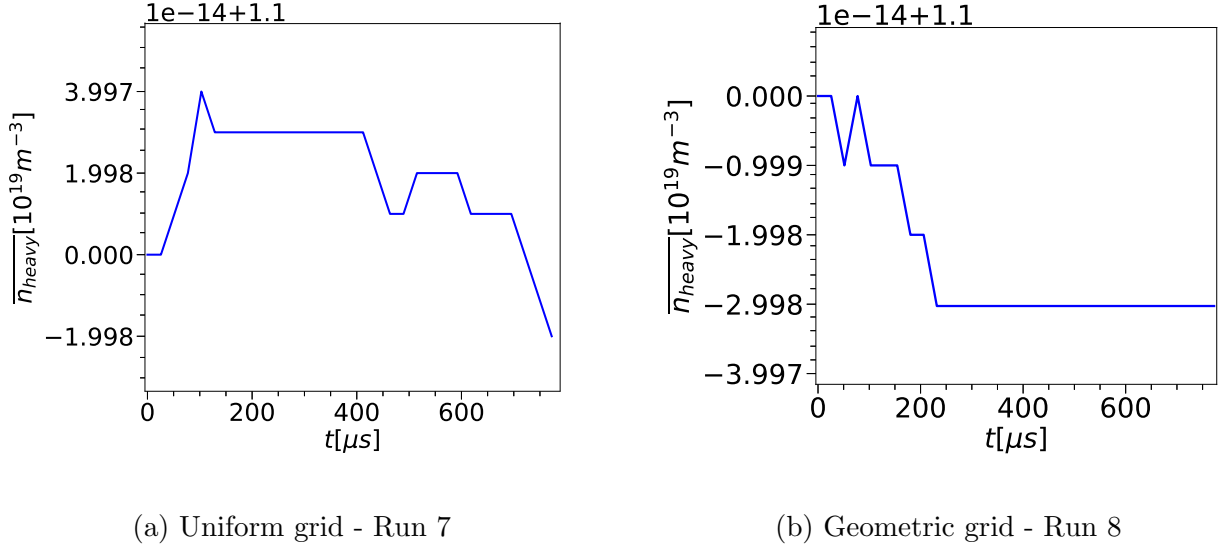


Figure 4.6: Evolution of total density in the two inelastic collision discretisation test runs.

hold up further into the non-local regime.

#### 4.8.2 Collisional-Radiative model and inelastic collision tests

The discretisation scheme for inelastic collisions developed for SOL-KiT is designed with three properties in mind - particle and energy conservation, as well as numerically consistent detailed balance. The tests that follow are meant to test the desired properties of both the inelastic collision operators as well as the accompanying collisional-radiative model.

**Conservation property tests** In order to test velocity grid dependence of the conservation properties two different runs were performed. The common run parameters are

$$n_0 = 10^{19} m^{-3}, \quad n_e = n_0, \quad n_1 = 0.1 n_0, \quad N_n = 30,$$

$$\Delta t = 0.5 t_0, \quad N_t = 30000, \quad N_v = 120, \quad T_0 = 5 \text{ eV}, \quad T_e = T_0,$$

where  $N_n$  is the total number of resolved hydrogen states. Both runs included only the inelastic electron-atom processes, and were performed with a low number of spatial cells. The first of the two runs (Run 7) used a uniform grid with  $\Delta v = 0.05 v_{th}$ , while the second (Run 8) used a geometric grid with  $\Delta v_1 = 0.01$  and  $c_v = 1.025$ .

Figure 4.6 shows the average heavy particle density ( $n_i + \sum n_b$ ) in the two runs. As can be seen the total error is of the order of  $10^{-14}$ , which is consistent with round-off errors. Similar results are obtained for the relative deviation of the total energy density  $E_{TOT} = 3n_e kT_e/2 + n_e \epsilon_{ion} + \sum n_b \epsilon_b$  from its initial value, where  $\epsilon_b$  is the  $1 \rightarrow b$  transition energy. This result is shown in Figure 4.7, where it appears that the geometric grid (Run 8) is performing somewhat better in the later part of the simulation, likely due to a finer velocity grid near the origin.

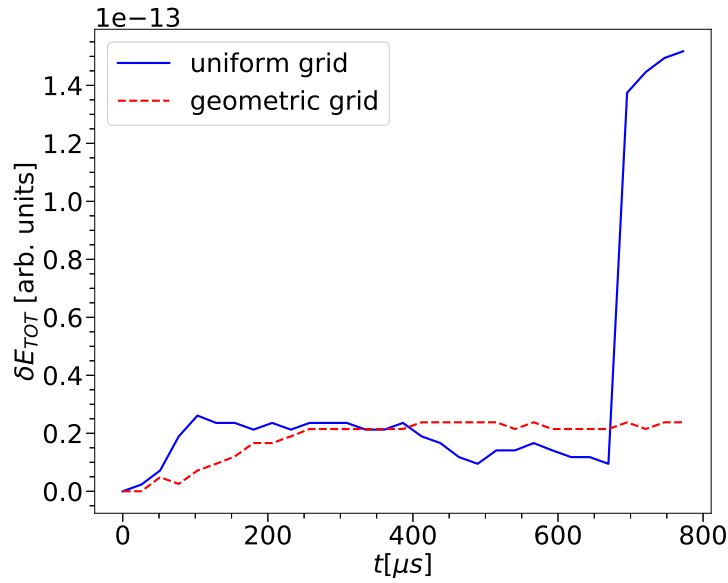


Figure 4.7: Relative change in total energy density in both electron motion and atomic states for the two inelastic collision discretisation test runs (Runs 7-8).

**Detailed balance test** In order to test the numerical detailed balance condition for the inverse processes the distribution function must be Maxwellian. To achieve this, electrons are treated as a fluid, effectively locking their distribution function into a Maxwellian. This simulation (Run 9) was performed with the same grid, normalisation, and initial conditions as the uniform grid run (Run 7) discussed above. The only difference was the timestep parameters being  $N_t = 1000$  and  $\Delta t = 100t_0$ . By the end of the simulation the atomic state distribution settled close to a Saha-Boltzmann equilibrium,

$$\frac{n_e^2}{n^{TOT} - n_e} = \frac{2}{g} \left( \frac{h^2}{2\pi m_e kT_e} \right)^{-3/2} e^{-\epsilon_{ion}/(kT_e)},$$

$$g = \sum_b 2b^2 e^{-(\epsilon_{ion} - \epsilon_b)/(kT_e)},$$

$$\frac{n_b}{n_1} = b^2 e^{-(\epsilon_{ion} - \epsilon_b)/(kT_e)},$$

$$n^{TOT} = n_e + \sum_b n_b$$

where the ionisation energy is  $\epsilon_{ion} = 13.6$  eV, and  $\epsilon_b = \epsilon_{ion}/b^2$ . The ionisation degree  $X = n_e/n^{TOT}$  relative error computed against the analytical solution for hydrogen was  $\delta X = 1.134 \times 10^{-8}$ , while the total density and energy errors at the end of the simulation were  $\approx 6 \times 10^{-14}$  and  $\approx 5 \times 10^{-14}$ , respectively.

Note that in all three runs discussed above all radiative processes were disabled, as those would mask any energy conservation processes in the first two runs, and would not allow for equilibrium in the detailed balance test.

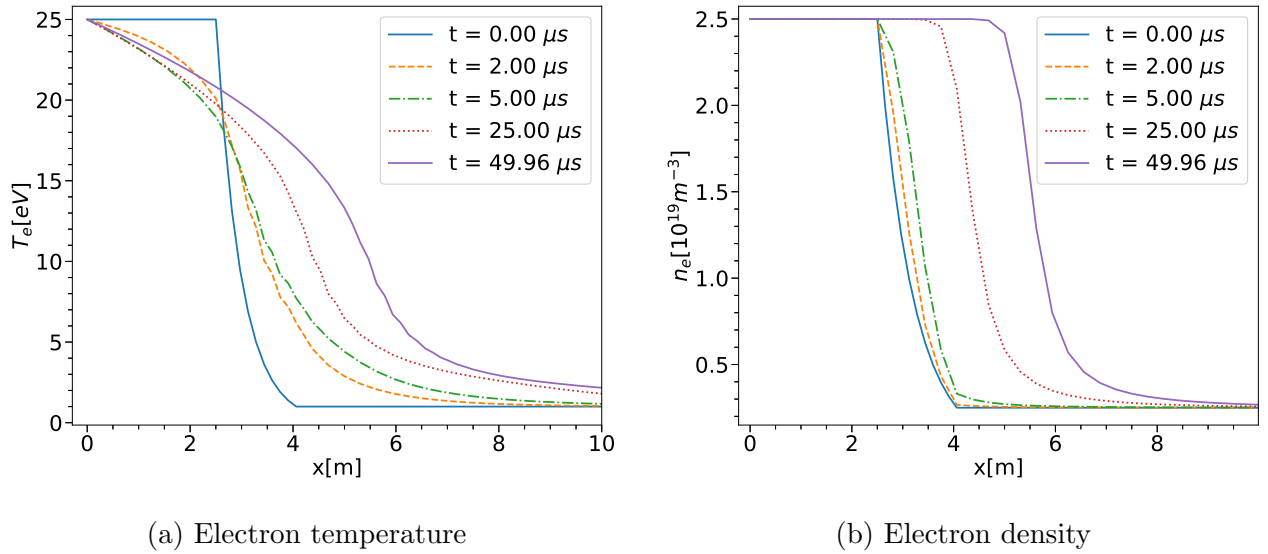


Figure 4.8: Evolution of temperature and density in reproduction of results from Allais et al. [3] (Run 10) - corresponds to Figures 1 and 2 from original paper.

**Integrated test** Finally, an integrated test (Run 10) was performed in order to test the full interplay of electron and neutral processes. An attempt was made to replicate, as closely as possible, the simulation performed by Allais et al.[3] using the code FPI. Parameters used in this run were

$$T_0 = 10\text{eV}, \quad n_0 = 2.5 \times 10^{19} \text{m}^{-3}, \quad N_n = 30, \quad n_{TOT} = n_0,$$

$$N_v = 80, \quad \Delta v_1 = 0.05 v_{th}, \quad c_v = 1.025, \quad l_{max} = 1$$

$$N_c = 64, \quad \Delta x = 5.536 x_0, \quad N_t = 16600, \quad \Delta t = 0.1 t_0,$$

amounting to a domain of length  $L = 20.31\text{m}$  and total simulation time  $t_{TOT} = 49.96\mu\text{s}$ . At  $x = 0$  the temperature is initialised to 25 eV, and the plasma is 100% ionised. From  $x = 2.5\text{m}$  to  $x = 4.06\text{m}$  the temperature drops exponentially to 1eV, while the ionisation degree drops to 10%. All inelastic collisions were enabled, as well as radiative processes, while ions and neutrals were left stationary as in the original paper. Boundary conditions were fixed to initial values. Figure 4.8 shows the evolution of electron temperature and density corresponding to Fig. 1. and Fig. 2. in [3]. Qualitative behaviour is recovered, while discrepancies of less than 10% are most likely caused by potential differences in the intialisation, as well as likely different spatial and velocity space resolutions (not reported in [3]). Another potential cause of discrepancy is the use of different databases in SOL-KiT compared to FPI.

### 4.8.3 Ion flow tests

The implementation of lab frame fluid ions requires the corresponding operators to be tested. This is presented below.

**Acoustic wave test** A standard test of ion advection, acoustic wave propagation was used to test the ion parallel velocity equation. The performed isothermal ion acoustic wave test (Run 11) had the following simulation parameters:

$$T_0 = 100\text{eV}, \quad n_0 = 10^{19} \text{m}^{-3}, \quad N_t = 6000, \quad dt = 0.01 t_0, \quad l_{max} = 1$$

$$N_v = 120, \quad \Delta v = 0.1 v_{th}, \quad N_c = 128, \quad dx = 0.0078125 x_0,$$

with the density and ion velocity initialised on a periodic grid of length  $L = x_0$  as

$$n(x) = n_0 + 0.01n_0 \sin\left(2\pi\frac{x}{L}\right), \quad u_i(x) = \frac{v_{th}}{6000} \sin\left(2\pi\frac{x}{L}\right).$$

Electron-electron collisions for  $l = 0$  and electron-ion collisions were turned on in the simulation. The density and ion velocity are presented at several points during the evolution of the acoustic wave in Figure 4.9. In order to evaluate the sound speed a sine function was fitted to the ion velocity profiles at different times, giving the value  $c_s = (1.001 \pm 0.013)c_s^{analytical}$ . Estimation of the error was performed conservatively, by taking the greatest deviation from the computed mean sound speed. Nonetheless, the obtained agreement is satisfactory even with the conservative error estimate.

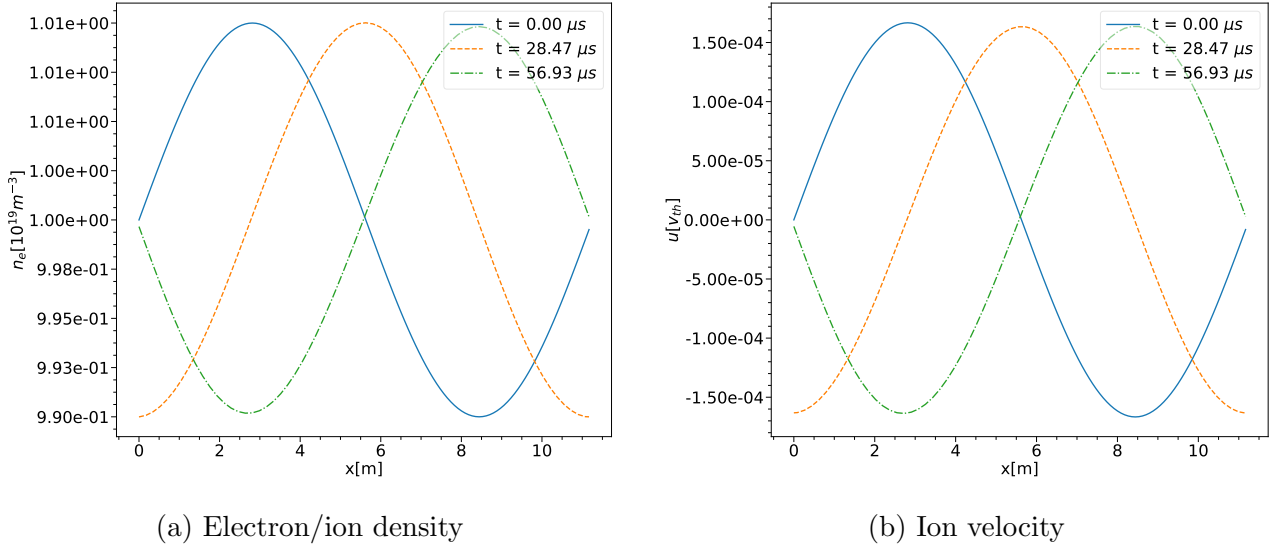


Figure 4.9: Evolution of density and ion velocity during the acoustic wave propagation test from Run 11. Graph and data analysis courtesy of Abetharan Antony.

**Charge-exchange friction test** To test the charge-exchange cross-section implementation, a set of runs (Set 2) with the following parameters was performed

$$T_0 = 10\text{eV}, \quad n_0 = 2.5 \times 10^{20} \text{m}^{-3}, \quad N_n = 1, \quad n_{TOT} = n_0, \quad n_{e,i} = n_0,$$

with the electrons and ions decoupled by turning the  $E$ -field and electron-ion collisions off. The only operator being tested was the charge-exchange friction term in the ion equation, and the total simulation time for all runs in the set was kept at  $500t_0$ . Ion flow velocity was initialised at

$u_i = v_{th}$ , and its value was compared to the analytical solution  $u(t) = u(0)/(1 + u(0)n_1\sigma_{CX,1}t)$  as the ions were slowed down by friction. The relative error of the evolved ion velocity is plotted in Figure 4.10 for different timestep lengths. It should be noted that the initial value of the ion velocity is unphysically high, and was used only for stress testing the operator, with velocities towards the end of the simulation being more in line with values observed in the SOL.

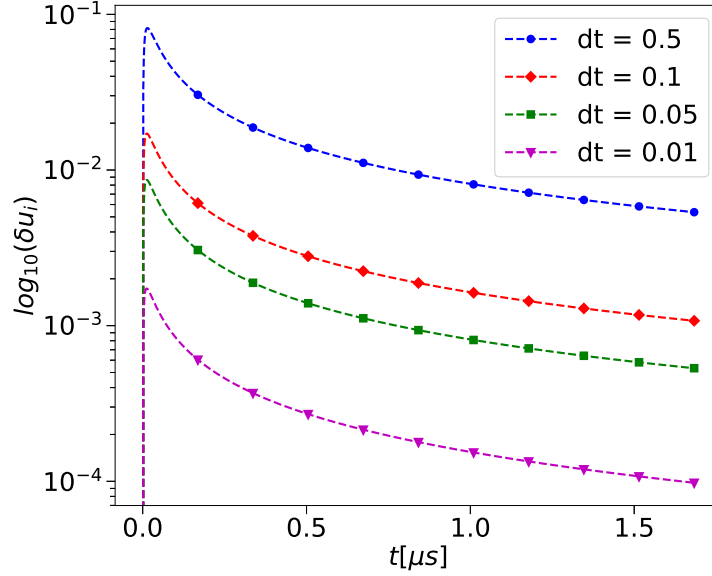


Figure 4.10: Relative difference between analytical and computed values during charge-exchange friction test for various timestep lengths - Set 2.

**Momentum loss in electron-ion collisions** As was noted in Section 4.5, electron-ion collisions with flowing ions (as well as electron-electron collisions in general) suffer from numerical loss of momentum. In the code, this loss is accounted for by transferring the lost momentum to the ions, conserving total momentum. However, a set of tests (Set 3) was performed to test the severity of this numerical “friction”, where only the electron-ion collision operator for  $l = 1$  was active. The common run parameters were

$$T_0 = 10\text{eV}, \quad n_0 = 2.5 \times 10^{19} \text{m}^{-3}, \quad N_t = 5000, \quad dt = 0.1t_0, \quad l_{max} = 1,$$

and a uniform velocity grid was utilised, with  $\Delta v$  ranging from  $0.02v_{th}$  to  $0.15v_{th}$ . The total length of the velocity grid was kept at or above  $6v_{th}$ . Both the ion and the electron flow velocities were initialised to  $u_e = u_i = 0.01v_{th}$ . If the electron-ion collision operator perfectly conserved

momentum, those flow velocities would have remained constant. Instead, at the end of each run they had equilibrated to values other than  $0.01v_{th}$ , while total momentum was conserved within tolerance.

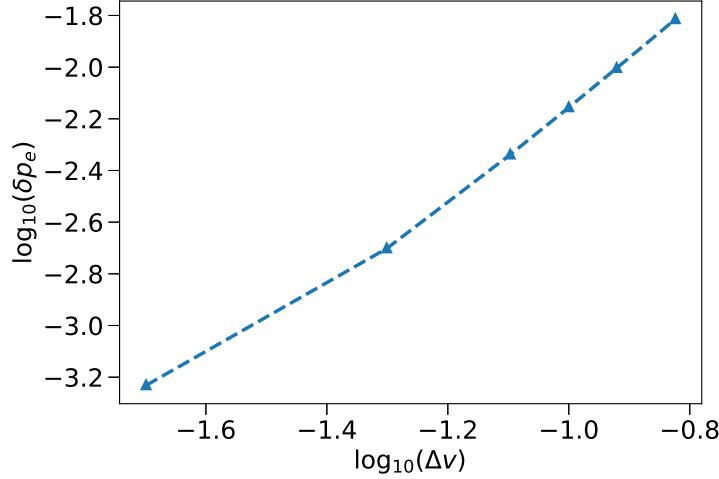


Figure 4.11: Relative error dependence on velocity grid resolution of the momentum due to electron-ion collisions based on runs from Set 3.

While electron-electron collisions were not tested in this set of runs, due to the similarity in operator form, it can be expected that the momentum error due to electron-electron collisions acting on  $l = 1$  is of the same order as the ones in Figure 4.11.

Figure 4.11 shows the relative deviation of the equilibrium electron momentum compared to the expected analytical value (based on the flow velocity remaining constant). The ion momentum error would be smaller than the electron one by the mass ratio, so electrons are the most affected. The used flow speed is also representative of SOL conditions, being of the same order of magnitude as typical sound speeds. In typical runs, one can thus expect momentum errors below 1%. However, when the electric field is turned on, these will manifest as a spurious electric field balancing the numerical friction.

#### 4.8.4 Divertor boundary condition tests

**Analytic limit convergence test** The first condition a cut-off logical boundary condition would need to satisfy is the analytical Maxwellian limit for the sheath properties. In order to test

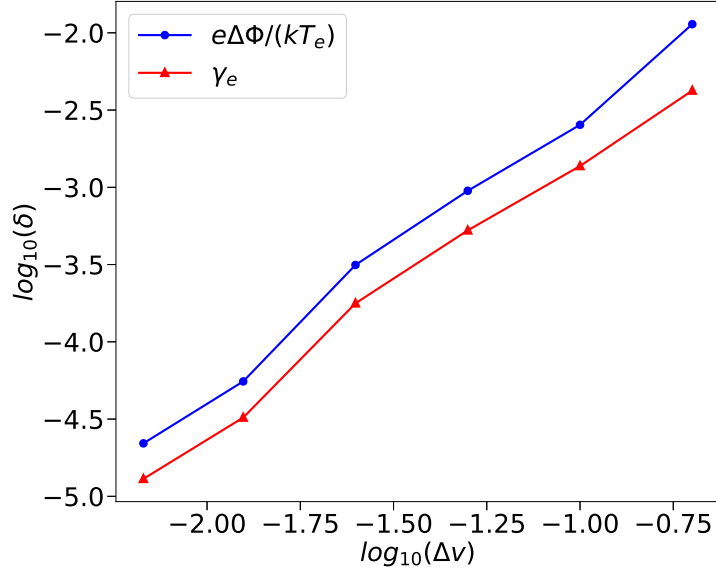


Figure 4.12: Relative error of computed sheath properties as a function of velocity grid resolution - Set 4.

this aspect of the operator, the cut-off procedure and calculation of the sheath heat transmission factor and potential drop were performed without evolving the initially Maxwellian distribution. A set of (effectively 0D) simulations (Set 4) with different velocity space resolutions (constant  $v_{max} = 6v_{th}$ ) was used to evaluate convergence. While the only operator active was the divertor boundary condition operator, the distribution function was not evolved (by setting  $\Delta t = 0$ ), and the operator was used merely to calculate what the cut-off distribution would be if the pre-reflection distribution is Maxwellian (see Section 3.5). The results of this test are shown in Figure 4.12, where it can be seen that both the sheath heat transmission coefficient  $\gamma_e$  and the potential  $\Delta\Phi$  are, even for the coarsest grid used, within a few percent of the analytical values

$$\frac{e\Delta\Phi}{kT_e} = -\frac{1}{2} \ln \left[ 2\pi \frac{m_e}{m_i} \left( 1 + \frac{T_i}{T_e} \right) \right],$$

$$\gamma_e = 2 + \frac{e\Delta\Phi}{kT_e}.$$

**High harmonic convergence test** In order to test convergence of the sheath properties in a driven system (with  $\Delta t > 0$  and driven by a fixed boundary condition) when the number of harmonics is varied a set of runs (Set 5) was performed with the following parameters

$$T_0 = 10\text{eV}, \quad n_0 = 2.5 \times 10^{19} m^{-3},$$

$$N_v = 80, \quad \Delta v_1 = 0.05 v_{th}, \quad c_v = 1.01,$$

with a short system  $L = 1x_0$  and  $N_c = 2$ . The velocity grid length was approximately  $6v_{th}$ . Electron-electron collisions were included only for  $l = 0$  while electron-ion collisions were on for all  $l > 0$ . A Maxwellian with  $T_e = T_0$  and  $n_e = n_0$  was imposed as a fixed boundary condition at  $x = 0$ . No atomic physics was included, as the fixed upstream boundary condition acts as a particle source. The temperature drop from the upstream cell to the target was in general low (around  $0.1 - 0.2$  eV), while the density developed at the target was considerably lower than the upstream density, dropping to  $n_e \approx 0.57n_0$ . This setup provided a scenario where the boundary condition operator was sufficiently stressed without entering a strictly collisionless regime. Simulations were run until the sheath properties equilibrated, and the results of the test are shown in Figure 4.13. Harmonic number was increased up to  $l = 25$ , and the relative changes in the sheath potential drop and heat transmission coefficient were tracked. Very quickly the change drops below 1%, before nonmonotonic behaviour is observed around  $l = 9$ . The cut-off velocities varied from  $v_c \approx 1.65v_{th}$  to  $v_c \approx 1.69v_{th}$ . While convergence appears slow, this is to be expected with such a sharply cut-off distribution being expanded in Legendre polynomials. Fortunately, even in this highly stressed scenario a relatively low number of harmonics  $l \leq 5$  seems to be enough to capture the physically important behaviour.

From Figure 4.13 one could guess the convergence rate of the sheath properties. If only  $l > 9$  is considered, the relative change in  $\gamma_e$  and  $e\Delta\Phi/(kT_e)$  is monotonic. Based on inspection of Figure 4.13, the following function was fitted to the sheath properties

$$|y_l - y_{25}|/y_{25} = a/l^2 + b, \tag{4.53}$$

giving  $a = 7.668 \times 10^{-2}$ ,  $b = 6.489e \times 10^{-5}$  for  $\gamma_e$  convergence, and  $a = 0.273$ ,  $b = -4.243 \times 10^{-4}$  for  $e\Delta\Phi/(kT_e)$  convergence. The fits are plotted in Figure 4.14, where they appear to fit the results well, pointing to a scaling close to  $|y_l - y_\infty|/y_\infty \propto l^{-2}$ .

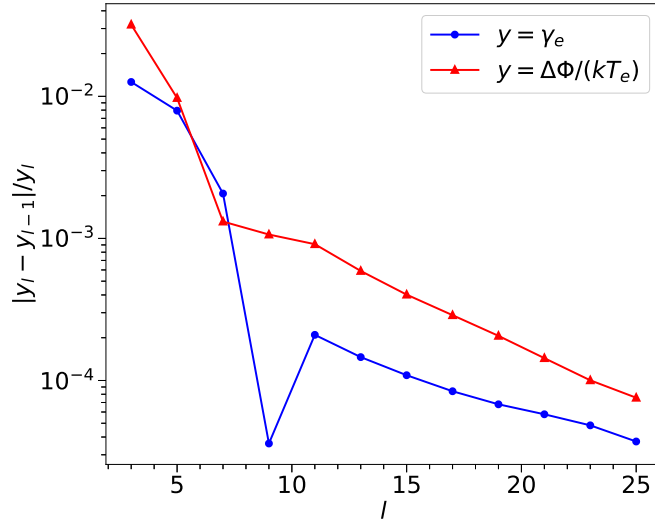


Figure 4.13: Relative change in sheath properties when increasing the number of harmonics in the simulation. Non-monotonic behaviour was observed around  $l = 9$ , causing the drop in relative change - Set 5.

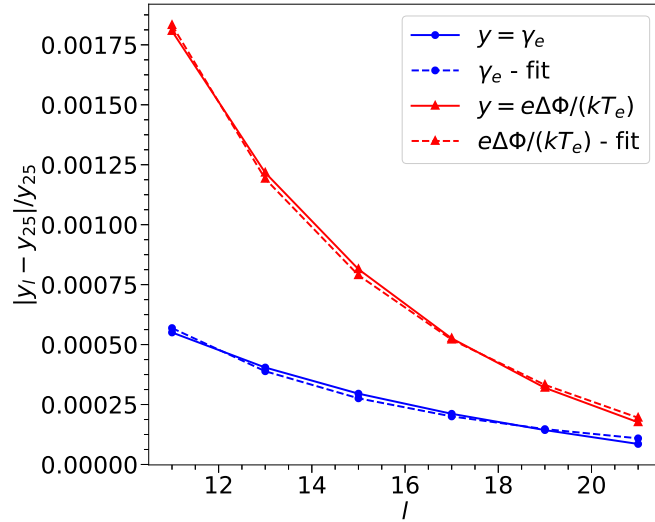


Figure 4.14: Fitting the function  $y = a/l^2 + c$  to  $|y_l - y_{25}|/y_{25}$  in order to estimate the order of convergence.

## 4.9 Summary and discussion

In this and the previous chapter, the SOL-KiT model and its implementation have been presented in detail. Both the fluid and the Legendre polynomial kinetic model for the electrons are outlined, with the focus being on the consistency between the models, allowing for cross-comparison to reveal kinetic effects more cleanly. The Legendre polynomial approach in particular is justified

by the simplification of collision integrals. Furthermore, a number of novel approaches and implementations have been incorporated into SOL-KiT, and those will be discussed in more detail here.

With collisions playing an important role in the determination of SOL regimes, it becomes necessary to pay close attention and devote care to their implementation. In SOL-KiT, Coulomb collisions are treated using standard approaches like the Chang-Cooper-Langdon scheme[115, 116, 117], as well as implementations borrowed from other VFP codes[100, 101]. However, a novel discretisation scheme was developed for inelastic electron-neutral collisions, which carry great importance in the SOL “kitchen” physics. With particles and energy conserved up to accumulated round-off error, and with detailed balance obeyed numerically, the new discretisation allows for performing equilibrium simulations without the worry that conservation properties might produce spurious sources and sinks. It is, however, worth noting that the inelastic collision operators, together with the Collisional-Radiative model, produce a stiff matrix due to the great disparity in timescales for various inelastic processes. While the fully implicit approach of SOL-KiT solves the problem of stability, this stiffness has the effect of accumulating round-off error when a large number of neutral states is used. For example, when  $N_n = 30$  the total number of collisional processes treated is 930, bringing the expected relative error up to an order of  $\approx 10^{-13}$ . The round-off nature of this error has been confirmed by performing slow runs with quad precision.

At the target sheath, SOL-KiT utilises the logical boundary condition [69], a standard condition used in kinetic codes for the SOL. However, due to the nature of the Legendre polynomial formalism, this condition becomes decidedly more complicated, and the first formulation of the logical boundary condition using Legendre harmonics has been presented and tested. Due to the sharp cut-off in the boundary condition distribution, one might expect that a large number of harmonics would be required for properly resolving the distribution. Fortunately, this is not the case, with Set 5 in the above benchmarking showing that a relatively low number of harmonics is sufficient to give reasonable estimates of the sheath properties. It has also been shown that the boundary condition, as implemented in SOL-KiT, reproduces analytical Maxwellian values up to finite grid errors.

Due to the fully implicit nature of SOL-KiT, it does not suffer from limitations imposed by the CFL condition. This allows computation of high harmonics in low velocity cells, which is not a possibility in explicit codes, like OSHUN[101]. As the boundary condition induces flows, a natural choice of frame is the lab frame, unlike the standard choice in VFP codes with flowing ions of using the ion rest frame[107, 106]. Together with inelastic collisions like ionisation affecting low velocity cells, the nature of electron-ion collisions with flowing ions makes the proper resolution of low velocity cells extremely important. The implicit framework thus supports two of the novel approaches, with flowing ion electron-ion collisions being the most affected due to the fact that the ion flow speed is much lower than the electron thermal velocity. For the implementation in the current version of SOL-KiT, the flowing ions are taken to be a cold beam. While finite ion temperature effects would potentially change the  $l > 0$  collision integral, it is likely that this effect would be negligible due to ion thermal velocities being small compared to the electron velocity grid scale. A much more important ion temperature effect would be the partial decoupling of ion and electron pressures and electron-ion energy exchange, as will be discussed in the next two chapters.

Most of the benchmarking runs were performed on a workstation including an Intel Xeon(R) CPU E5-2630 v3 @ 2.40GHz with a maximum of 16 threads. While the detailed analysis of computational efficiency of the code is yet to be performed, following a number of necessary optimisation updates, it is worth quickly noting some of the computational times for runs presented in this chapter. The majority of runs was performed with the full 16 threads utilised, and the run time varied between 6 minutes for the local Spitzer-Härm tests to around 18.5h for the full scale reproductions done in Run 10. The neutral collision conservation property tests were performed on a single thread, and took just under 7h. The production run computational costs will be commented on in the next chapter. In general, the two bottlenecks identified so far are some aspects of the matrix construction, specifically the constructions of electron-electron collision operator submatrices for  $l > 0$  and inelastic collision operators, as well as the matrix solver. Bundling of the neutral states is a planned extension of the code, which should address the main bottleneck - the large number of inelastic collision operators constructed during each iteration.

Further additions and improvements to the code are considered in the results chapters that follow, with the discussion in the context of physical regimes and simulation results.

# Chapter 5

## Simulations of SOL equilibria and transients

### 5.1 Setup and motivation

The interaction of transients with detachment is currently an important research concern, informing future reactor design. Parallel energy and particle transport plays a key role in characterizing this interaction, and kinetic effects in parallel transport are expected to be present[1]. As was discussed in Section 2.6, a number of numerical studies have been performed in order to understand kinetic effects in both equilibria and transients, ranging from simulations with PIC [80] and finite difference codes [72, 2, 87] to comparative studies with fluid codes[94].

An important aspect in the above studies is the understandable focus on machine-specific conditions. For example, Havlíčková et al.[94] simulate convective ELMs in JET, Chankin et al.[87] simulate equilibria in a JET H-mode, while Batishchev et al.[2] simulate Alcator C-mod and TdeV equilibria and ELMs. Systematic parameter scans aimed at uncovering fundamental properties of kinetic effects in the SOL are difficult to find in the literature. As such, a scan in input power was performed using SOL-KiT, utilising the code’s capability to self-consistently model both fluid and kinetic electrons. This chapter is devoted to the basic analysis of that scan, covering both equilibria and transients, after introducing the simulation setup in detail.

In determining the parameters for the runs presented here, the two main considerations

were:

- Working in medium size tokamak (MST) relevant parameter space,
- Capturing both detached and attached plasma states.

The chosen parameters for the simulations sets were thus taken as follows. While on the lower end for MSTs, the line-averaged total (plasma and neutral) density was set to  $\langle n_{tot} \rangle_L = 1 \times 10^{19} m^{-3}$  by utilising 100% recycling ( $R = 1$ ), providing a compromise between relevant densities and simulation time, which is governed by collisionality. The simulation domain length was set to  $L = 10.18m$ , representing half of the total connection length. The heating region length, interpretable as the region of upstream external heating and cross-field energy transport, was set to  $L_h = 3.75m$ . Neutral atoms produced at the target via recycling are given a temperature of  $T_n = 3eV$  (mimicking Franck-Condon enhancement [12]). This simulation setup is shown in Figure 5.1. Finally, in order to capture a wide range of plasma regimes, the effective input/heating power flux  $W_h$  was varied from  $1MW/m^2$  to  $6MW/m^2$ .

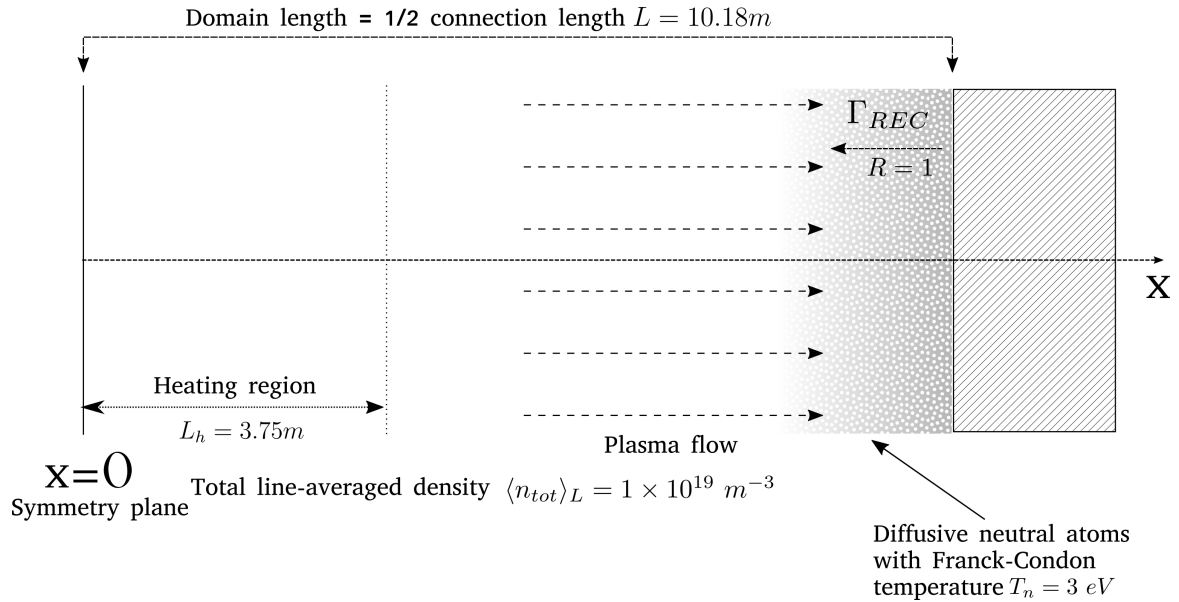


Figure 5.1: Diagram of the simulation domain with main parameters included.

The general numerical parameters of the simulations, as defined in Chapter 4, are:

$$T_0 = 10eV, \quad n_0 = 2.5 \times 10^{19} m^{-3}$$

$$N_v = 80, \quad \Delta v_1 = 0.05v_{th}, \quad c_v = 1.025,$$

$$N_c = 64, \quad \Delta x = 8.5x_0, \quad \Delta x_L = 0.5x_0,$$

$$l_{max} = 1, \quad N_n = 30, \quad N_h = 9,$$

amounting to a logarithmic spatial grid of length  $L$ , and a velocity grid of length  $\approx 12v_{th}$ . This allows for enhanced resolution near the divertor target and the velocity space origin, while the upstream and velocity space tail are still captured, but without the unnecessary high resolution.

## 5.2 Equilibrium results

With the simulation setup described above, it is possible to reach equilibrium by running SOL-KiT for a long enough time. The relevant scale is that of multiple sonic transition times along the length of the SOL, as the acoustic transients dampen throughout the simulation. For runs with fluid electrons, where the timestep is not limited by the computational stiffness of collisional operators, it is relatively easy to run SOL-KiT for long enough to equilibrate in a reasonable amount of time. When electrons are treated kinetically, however, reaching the equilibrium becomes a costly affair, especially for lower input powers, when the collisional times being resolved are much shorter than the timescale of acoustic transients. Therefore, in order to obtain kinetic equilibria one has two choices. The first choice is the obvious brute force approach in simply waiting for the kinetic simulations to equilibrate over a long time. This was the original approach in the presented study, and it worked well for attached plasma cases, where the collisional timesteps were long enough to allow for relatively quick convergence on the fluid timescale. In order to speed up the convergence, particularly for the detached cases, an iterative coupling approach was developed. In this way, the kinetic mode of the code is run first, providing transport coefficients for the fluid model, which is then run to resolve fluid scale phenomena efficiently. This approach is then repeated until the transients become weak enough to be ironed out with a kinetic run of reasonable length. Details of the coupling scheme are presented in Appendix E. The convergence criterion used was that the local Mach number in the upstream region does not exceed  $M = 5 \times 10^{-3}$ , determined by inspection.

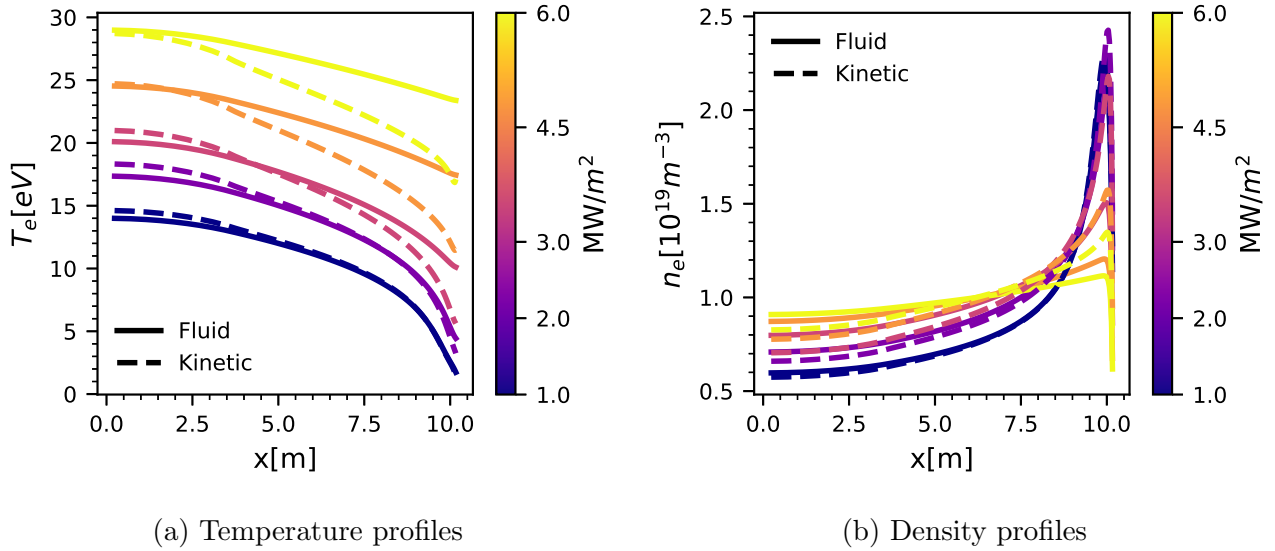


Figure 5.2: Temperature and density profiles for several different input powers in the scan, comparing kinetic and fluid equilibria.

Comparisons of equilibrium temperature and density profiles for runs performed in fluid and kinetic mode are shown in Figure 5.2. As expected, in both fluid and kinetic cases, both the density and temperature profiles flatten as input power is increased. However, it is immediately evident that the kinetic profiles retain their steepness to a higher degree throughout the power scan. This is the consequence of heat flux suppression, presented in Figure 5.3, through the ratio of the kinetic conductive

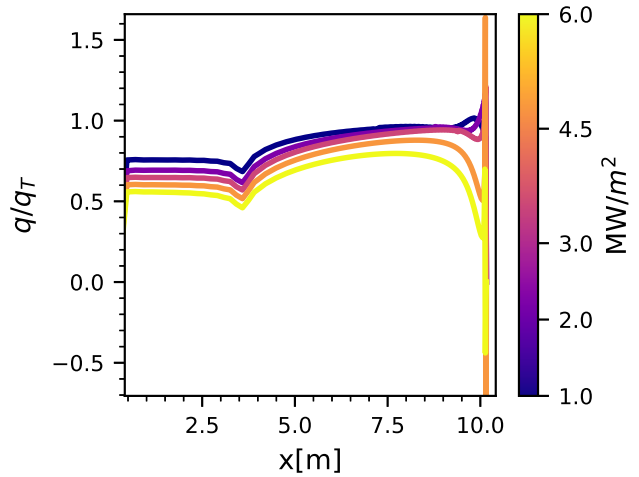


Figure 5.3: Ratio of calculated conductive heat flux to classical Spitzer-Härm value.

heat flux to that calculated using the same temperature profile and the classical Spitzer-Härm conductivity (here labeled  $q_T$ ). Heat flux is systematically suppressed upstream, while weak enhancement is visible close to the target for lower input powers.

At this point, several things can be noticed in kinetic simulations shown in Figures 5.2 and 5.3. The first is the heating artefact upstream, leading to a change in density and temperature gradients, as well as a dip in  $q/q_T$ . This is most likely due to the isotropic nature of the heating

operator. The other artefact that must be noted is the temperature uptick close to the divertor target. While not visible on the scale in Figure 5.2 it is present in Figure 5.3 as negative ratios. A similar phenomenon is observed by Mousseau[120] when ions are treated as cold. Runs with SOL-KiT show that this artefact is strongly affected by the ion mass, and together with the result from Mousseau, this suggests that the  $T_e = T_i$  approximation is to blame, as it leads to wrongly calculated ion pressure gradients, influencing the electric field. Further development work is necessary to improve on this approximation.

In order to further illustrate the differences between the kinetic and fluid model, a simple Two-Point Model (2PM) [12] result for the temperature where an input heating flux  $q_{in}$  is distributed along a heating length  $L_h$  can be written as

$$T_u = \left[ T_t^{7/2} + \frac{7 q_{in}(L - L_h/2)}{2 \kappa_e} \right]^{2/7}, \quad (5.1)$$

where  $\kappa_e$  was calculated by taking a Coulomb logarithm of 12. To compare the 2PM with the fluid and kinetic electron temperature simulations  $T_u^{7/2} - T_t^{7/2}$  is plotted as a function of input power in Figure 5.4. The fluid results

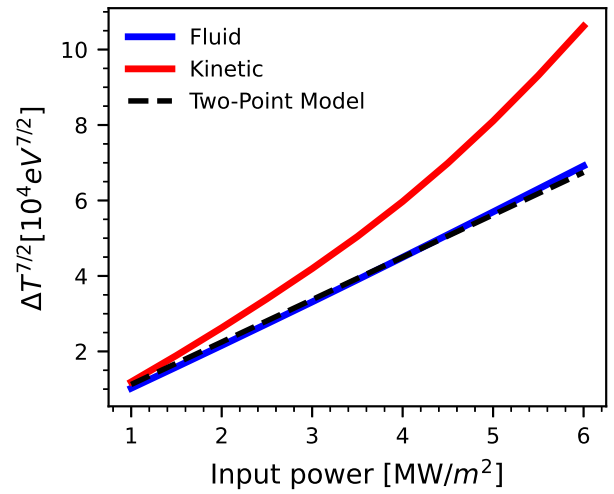


Figure 5.4:  $T_u^{7/2} - T_t^{7/2}$  as a function of input power for the simulated equilibria. The 2PM (equation (5.1)) result is given as the dashed line, and seems to agree well with the fluid simulations.

appear to agree well with the 2PM, although the densities (as shown in Figure 5.2) do not obey the 2PM, due to the presence of spatially resolved sources and sinks, and the resulting change in pressure balance. The slope in the kinetic simulations systematically increases, which points to a reduction in the effective heat conductivity  $\kappa_{e,eff} < \kappa_e$ . This is another manifestation of flux suppression.

Another way to look at the presence of kinetic/non-local effects is by looking directly at the distribution function, and comparing it to a Maxwellian distribution. For this purpose, the  $f_0$  harmonic is plotted in Figure 5.5, compared to Maxwellians with equivalent density

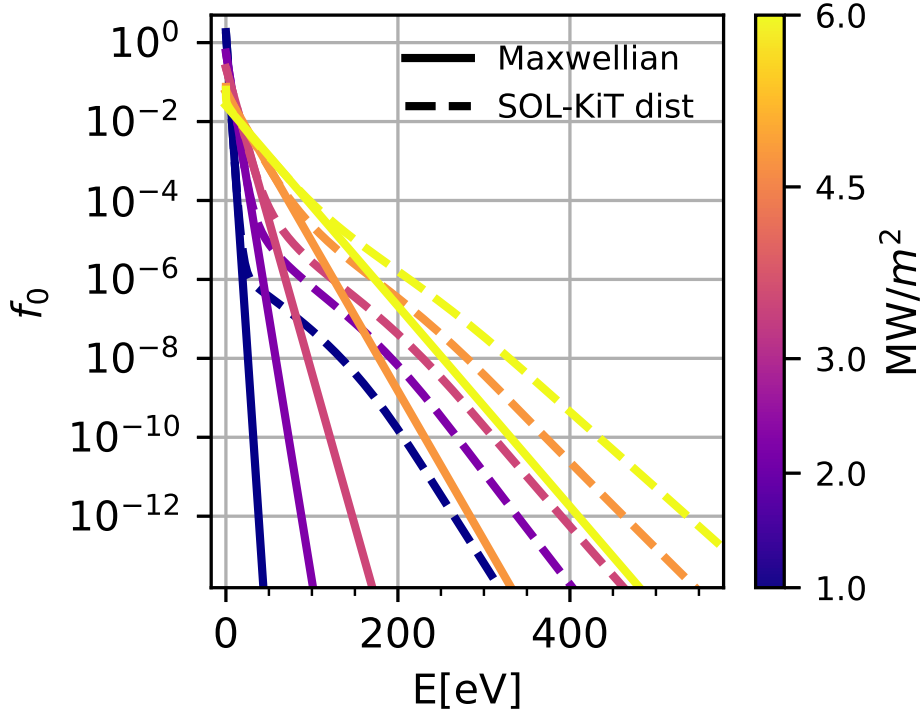


Figure 5.5: The  $l = 0$  harmonic near the target sheath for several input powers in kinetic runs. The solid line shows a Maxwellian with the same temperature and density as that calculated from  $f_0$ .

and temperature. Several input powers are shown, and the spatial point is the last cell before the divertor target. A “hot” tail of fast electrons can be seen in  $f_0$ . These fast particles originate from upstream and produce the characteristically non-Maxwellian shape of the electron distribution. Fast (tail) electrons can carry a substantial amount of the total heat flux at a given spatial point. This flux is given by

$$q_{fast} = \frac{m_e \int_{v_{thresh}}^{\infty} f_1(v) v^5 dv}{6}, \quad (5.2)$$

where  $E_{thresh} = m_e v_{thresh}^2 / m_e$  is chosen as the threshold energy, such that any electron with energy greater than that is counted as a tail electron. The following criteria can be used to determine that threshold

$$E_{thresh} \geq 5T_e \quad (5.3)$$

$$|f_0(v_{thresh}) - f_0^M(v_{thresh})| / f_0(v_{thresh}) \geq 0.1, \quad (5.4)$$

Table 5.1: Percentage of the heat flux carried by tail electrons in Figure 5.5

| $q_{in}$ [MW/m <sup>2</sup> ] | 1     | 2     | 3     | 4.5   | 6     |
|-------------------------------|-------|-------|-------|-------|-------|
| % $q_{fast}$                  | 21.44 | 38.61 | 51.33 | 61.87 | 65.15 |
| $E_{thresh}$ [eV]             | 13.4  | 27.6  | 41.7  | 72.3  | 100.8 |

where  $f_0^M$  is the equivalent Maxwellian to  $f_0$ . The first criterion simply asks that the electrons (loosely) correspond to heat-carrying electrons (as defined in Section 2.6). The second criterion makes sure that just those electrons where  $f_0$  departs from Maxwellian are counted, tracking only the tails in Figure 5.5. The percentage of heat flux carried by the tail electrons as well as the threshold energies are given in Table 5.1. Looking at the table, it can be seen that even the lowest power equilibrium has fast tail electrons carrying a non-negligible fraction of the heat flux. The increase in the percentage of fast electron heat flux as input power is increased corresponds to the steeper temperature profiles, as seen in Figure 5.2, further showing their correlation with kinetic effects.

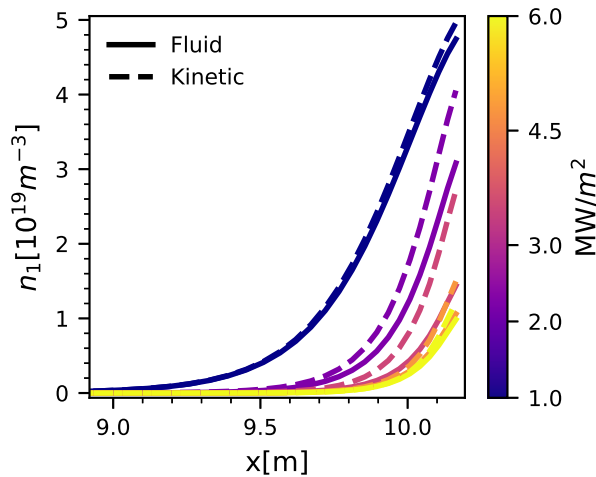


Figure 5.6: Deuterium ground state profiles for several different input powers, close to the target.

As was noted in the previous section, investigating kinetic electron effects in detachment is one of the principle concerns of this study, informing the power scan bounds. It is already possible to infer that detachment-like behaviour is present for lower input powers from the temperature profiles presented in Figure 5.2, as the target temperature drops well below 5 eV. To confirm detachment, one can look at the density profiles of the deuterium ground state, to see whether a significant amount of neutrals accumulates for lower input power

fluxes. This is plotted for both the fluid and the kinetic electrons in Figure 5.6. It is evident from the neutral density profiles that at lower powers a cloud of considerable density forms. The kinetic runs show a higher density of neutrals, owing to the reduced target temperatures.

The classic detachment criterion, target flux rollover (see Section 2.2.4), is defined for an

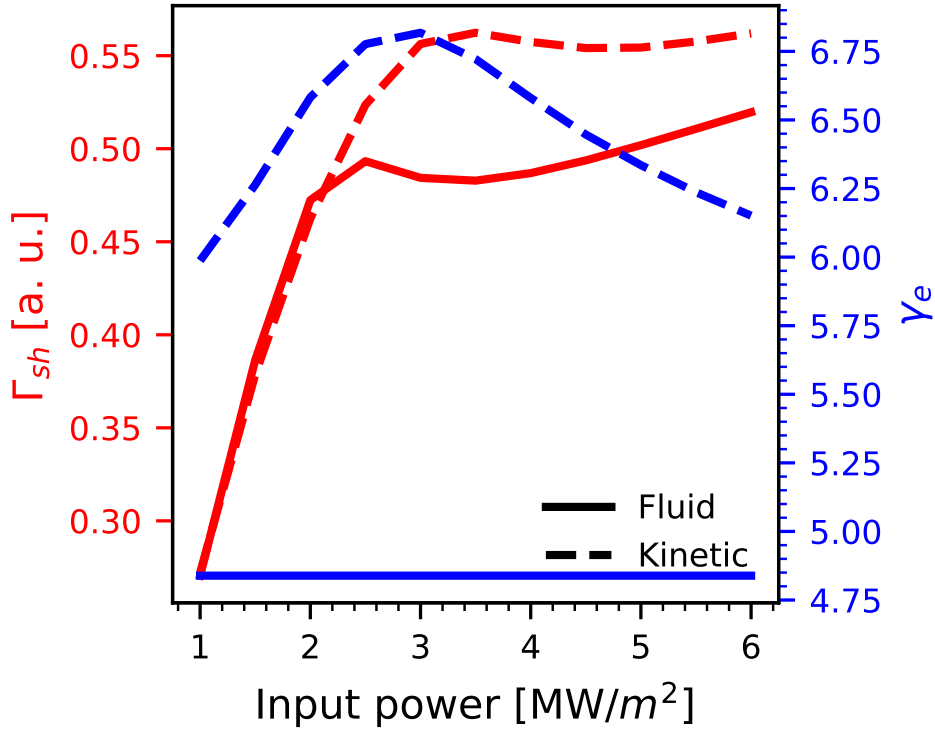


Figure 5.7: The particle flux and the electron sheath heat transmission coefficient into the target sheath as a function of input power.

upstream density scan, with rollover occurring as density increases. However, given that the performed study includes a power scan, and not a density scan, looking for rollover is slightly more complicated, but still possible. Two differences must be kept in mind. Firstly, flux rollover in a power scan would occur as input power is lowered. Secondly, the power scan in this study was performed with a constant total line-averaged density. As such, an increase in power increases the plasma density, due to increased ionisation, leading to increased target fluxes at high powers, since the target flux (in the 2PM) scales as  $\Gamma_t \propto n_u^2$  [12]. This added non-monotonicity complicates the interpretation of potential rollover, as it might mask the initial increase in plasma flux as input power is dropped and target plasma density increases. However, in the case presented here, detachment onset rollover is still visible, as shown in Figure 5.7, even though the flux increase due to enhanced ionisation is visible at high input powers. Both electron models roll over at low input powers, with the kinetic case rollover occurring at  $3.5 \text{ MW/m}^2$ , while the fluid runs roll over later, at  $2.5 \text{ MW/m}^2$ . This is likely due to increased steepness of the temperature profile in kinetic runs, as described above, allowing for lower target

Table 5.2: Possible combinations of equilibria and perturbations based on equilibrium and perturbation physics used.

|                     | Fluid perturbation | Kinetic perturbation |
|---------------------|--------------------|----------------------|
| Kinetic equilibrium | NA                 | kinetic on kinetic   |
| Fluid equilibrium   | fluid on fluid     | kinetic on fluid     |

temperatures in kinetic equilibria.

Finally, an important aspect of kinetic SOL runs is the ability to calculate the sheath heat transmission coefficient (see 2.12), plotted in Figure 5.7 as a function of input power in kinetic runs. In fluid runs it is set to  $\gamma_e = 2 - 0.5 \ln(2\pi(1 + T_i/T_e)m_e/m_i)$ , which for deuterium and  $T_e = T_i$  results in  $\gamma \approx 5$ . Around  $3.0\text{MW}/m^2$  the coefficient experiences a rollover-like effect. This behaviour can be explained as follows. In the low input power limit collisions can be considered dominant, and the fluid model works well, so the sheath heat transmission coefficient tends to its classical limit. When no gradients are present, such as in a high input power attached plasma regime, it can again be expected to have the coefficient return to  $\approx 5$  due to the electron distribution at the target being essentially the upstream Maxwellian. Accordingly, if there is any change in  $\gamma_e$  during a power scan, rollover-like behaviour at an intermediate input power is to be expected. Similar non-monotonic behaviour during a pure collisionality scan was observed in both BIT1[80] and KIPP [5] simulations.

### 5.3 Transient simulations

As was noted in the introduction to this chapter, the interaction of transients with detachment is a major research concern in the area of SOL modelling. With that in mind, and with a set of equilibria ready for perturbation, the following approach was taken in simulating transients in the SOL. Firstly, the choice was made to simulate conductive transients, represented by a temporary increase in input power flux. This was practically achieved by taking the above equilibria as initial conditions, and setting the heating flux to  $45\text{MW}/m^2$  for  $\approx 10\mu s$ . The perturbations were relaxed for a further  $\approx 10\mu s$  by resetting the input power to the original value. The choice to take  $45\text{MW}/m^2$  as the perturbed power flux comes from multiplying the  $4.5\text{MW}/m^2$  equilibrium input power by 10 (similar to an approach taken in ALLA[2]). After

that, it was decided to keep the same perturbation power, with the effective multiplier for other equilibria being still on the order of 10, in order to explore the response of different equilibria to effectively the same perturbation. Since both the kinetic and fluid equilibria are well into the attached regime above an input power of  $4.5\text{MW}/m^2$ , that case is treated as a representative attached case, and higher powers are not used in the perturbation study. In this way, both detached and attached plasma responses are investigated. Finally, the timestep in transient simulations is set to  $\approx 3ns$ , allowing the collisional processes to be resolved.

Since SOL-KiT allows using fluid initial conditions for kinetic runs, it is possible to launch kinetic perturbations on fluid backgrounds. Even with the coupling presented in Appendix E used for obtaining kinetic equilibria, using pure fluid profiles as initial conditions would significantly reduce run time. This trade-off between speed and accuracy is explored below, considering the three possible combinations of equilibria and perturbation physics (presented in Table 5.2).

Figure 5.8 shows the temperature profile evolution throughout the perturbation when using the lowest power,  $1\text{MW}/m^2$ , equilibrium. Here, the initial temperature profiles for the fluid and kinetic electron equilibria agree well. However, as the perturbation advances, it is evident that the heat conduction in the fluid case is stronger. This is most readily seen in

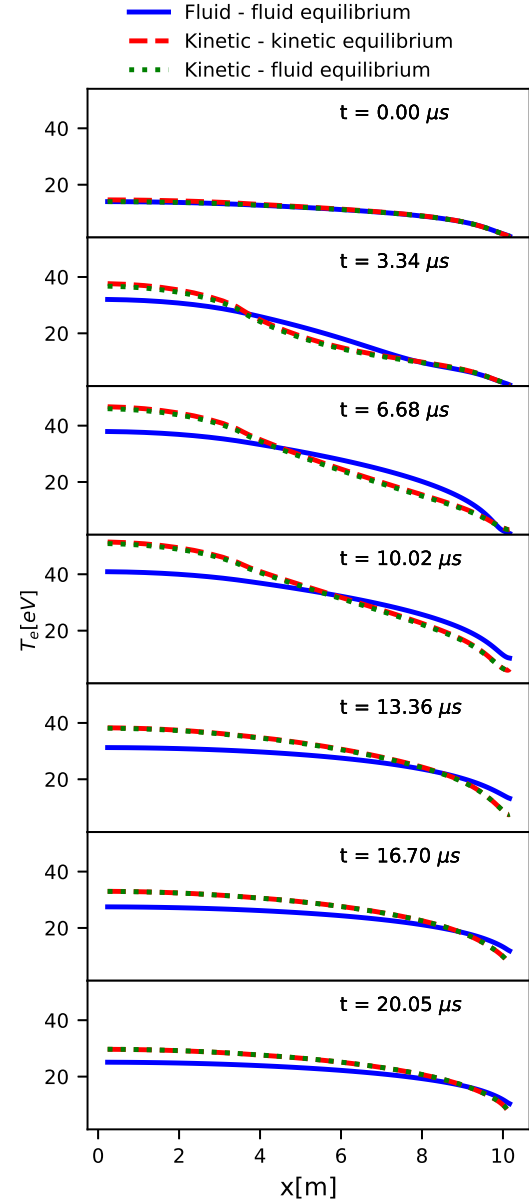


Figure 5.8: Temperature profile evolution for perturbation launched on the  $1\text{MW}/m^2$  background.

the much lower upstream and higher target temperatures, as opposed to the kinetic runs, where heat flux suppression leads to a hotter upstream, and a colder divertor target during and after the heating phase. The two kinetic simulations, both on the fluid and kinetic backgrounds, agree well. An agreement between them in this case is expected, as the profile differences between fluid and kinetic electron equilibria for the case of the lowest input power are not strong.

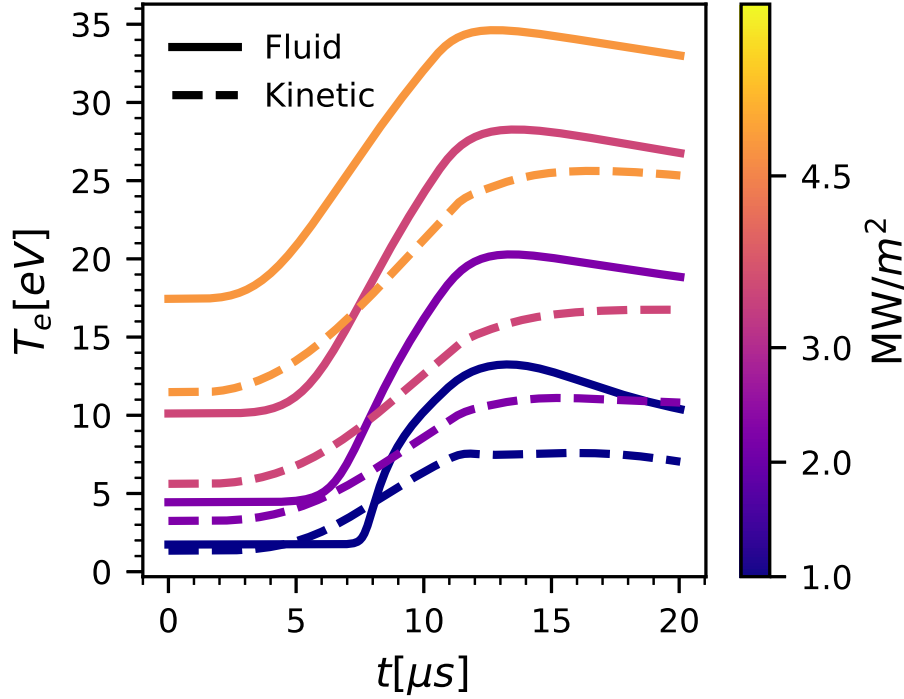


Figure 5.9: Evolution of the temperature perturbation at the target for the several input powers. Presented are both fluid perturbations (on fluid background) and kinetic perturbations on kinetic background.

Target temperature evolution is plotted in Figure 5.9, for several equilibrium input powers. Both the fluid perturbations (on fluid background) and the kinetic perturbations on kinetic background are shown for contrast. Peak target temperatures are systematically higher in the fluid case, with the lowest power equilibrium showing the greatest reduction (a factor of two), as could have been inferred from Figure 5.8, as well. Another effect, to be explored in more detail in the next chapter, is the presence of preheat in kinetic simulations, i.e. heating due to fast particles not accounted for in the fluid model. The point in time when the target temperature starts rising in the detached kinetic case is almost  $5\mu\text{s}$  before the corresponding time in the fluid simulation, indicating the presence of fast particles.

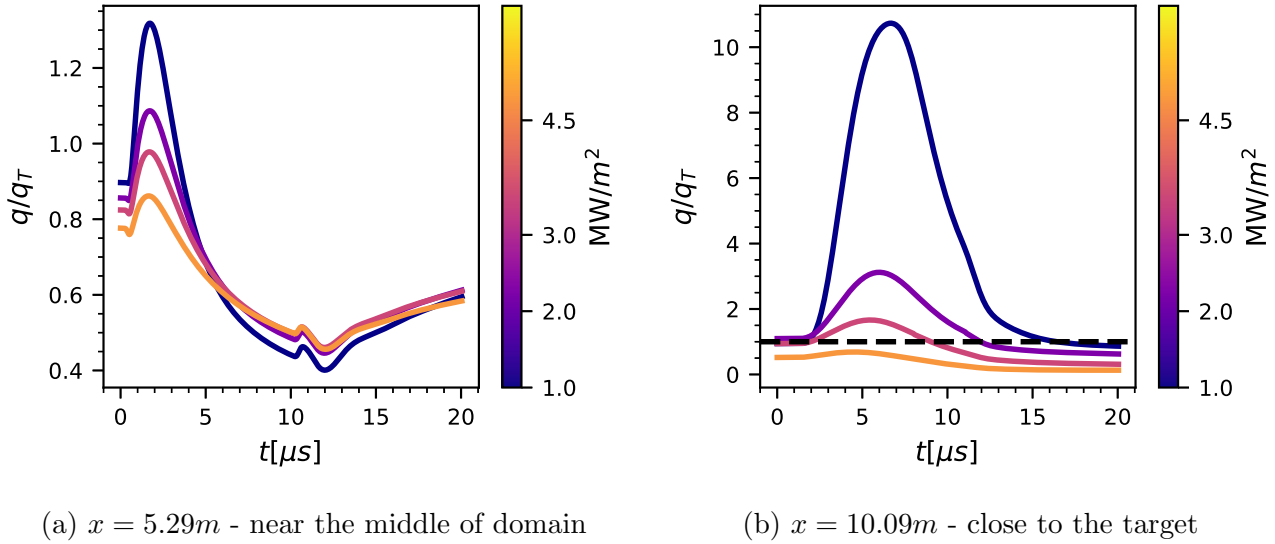


Figure 5.10: Evolution of heat flux ratio for two locations in the SOL and for different equilibrium input powers. Dashed line in (b) shows  $q/q_T = 1$ .

To explore kinetic effects in transients further, the same approach is taken as during the equilibrium analysis, and  $q/q_T$  is plotted in Figure 5.10 for two locations in the SOL, and for various equilibrium heating powers. The plotted transients were run on a kinetic background, and the locations were chosen to represent the middle of the domain and a point close to the target. Figure 5.10a shows that, after a short period of weak enhancement, the middle of the simulation domain experiences strong heat flux suppression. On the contrary, as seen in Figure 5.10b, strong enhancement, reaching  $q/q_T = 10$ , is observed close to the target for most of the simulation. It is also of note that the lowest power equilibrium is apparently the most susceptible to these kinetic effects. This is likely due to the much larger energy difference between the local cold electrons of lower power equilibria and the much hotter perturbed electrons coming from the upstream.

To visualise the contrast between hot and cold electrons during the transient, the evolution of the  $l = 0$  harmonic in the last simulation cell for the perturbation on the kinetic  $1\text{MW}/\text{m}^2$  equilibrium is plotted in Figure 5.11. As expected, the hot electron tail grows during the perturbation becoming more pronounced.

As Havlíčková et al.[94] remark, the evolution of the sheath parameters during transients is not well captured by fluid codes, leading to the need to change the ratios of electron and ion

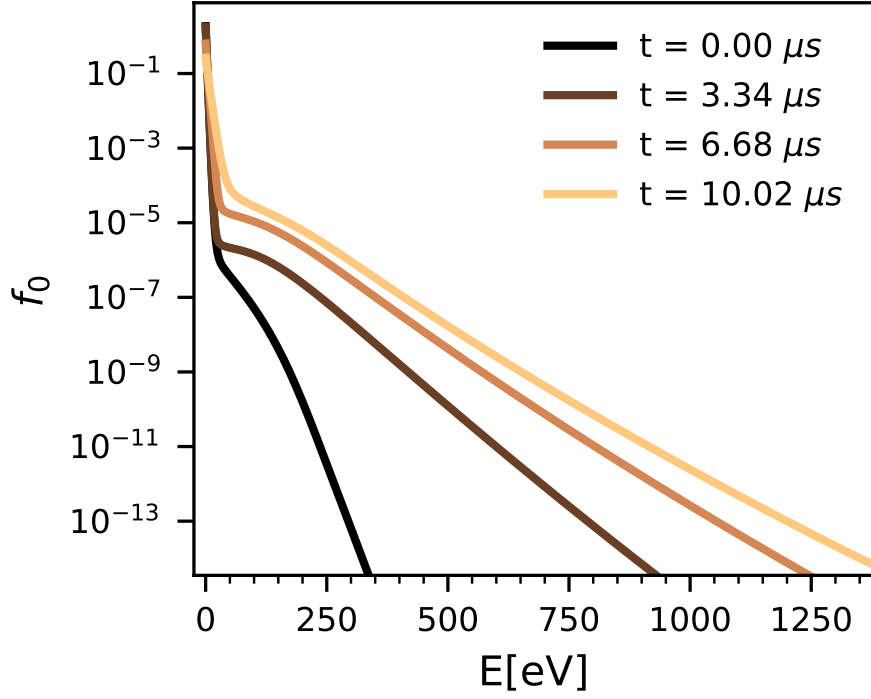


Figure 5.11: Evolution of the  $l = 0$  harmonic near the boundary during the perturbation on the  $1\text{MW}/\text{m}^2$  input power background.

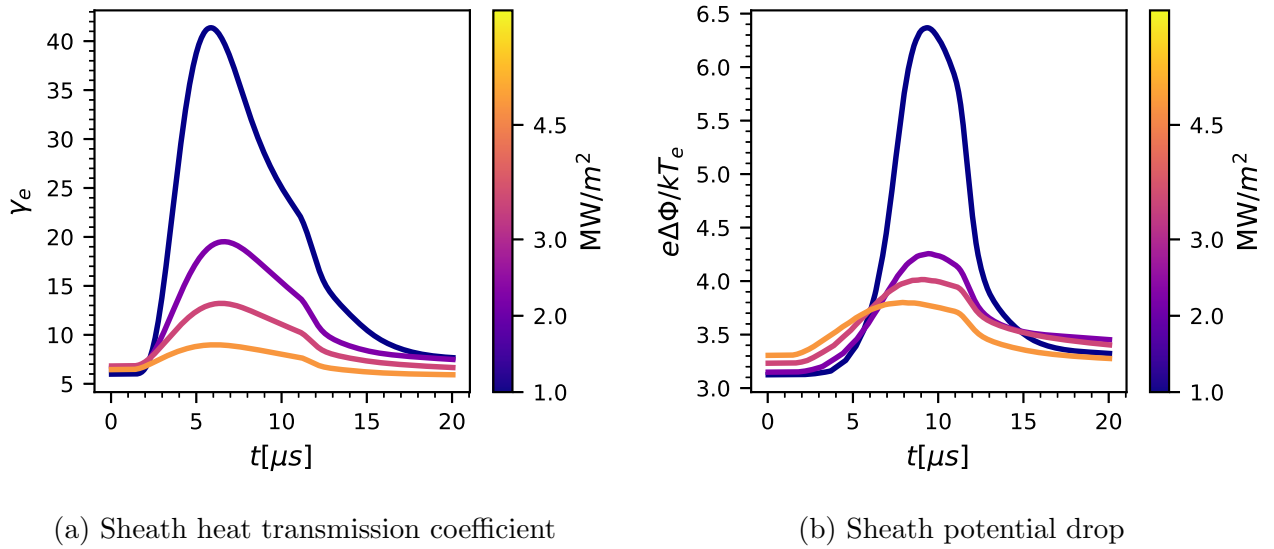


Figure 5.12: Evolution of the sheath heat transmission coefficient and potential drop during the perturbation for several different equilibrium powers on kinetic equilibria.

heating in fluid modelling (see Section 2.6). Since SOL-KiT can calculate both the sheath heat transmission coefficient and the sheath potential drop, it is possible to observe the evolution of these two parameters. The evolution of both of these quantities is plotted in Figure 5.12 for perturbations on kinetic equilibria.

Firstly, it can be seen that the sheath heat transmission coefficient  $\gamma_e$  can vary significantly during the perturbation, up to almost a factor of 8 for the strongest variation. Furthermore, the same sensitivity of lower initial power runs to kinetic effects observed in Figure 5.10 is present in Figure 5.12a as well. Similarly, the evolution of the sheath potential drop is plotted in Figure 5.12b. The potential varies up to around a factor of 2 compared to the classical result of  $\approx 3.0$ , less than  $\gamma_e$ .

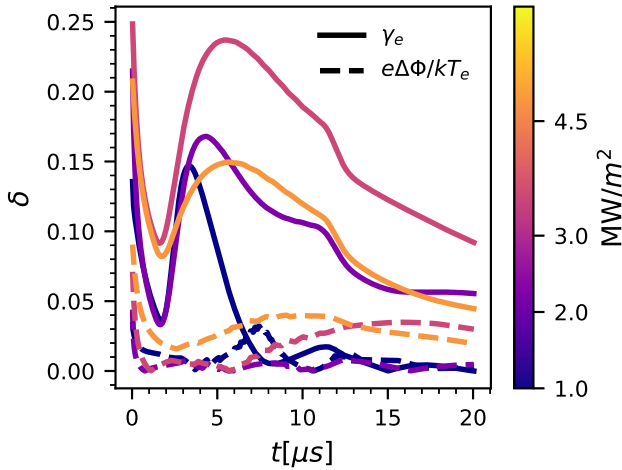


Figure 5.13: The relative deviation of the sheath properties between fluid and kinetic equilibria used as initial conditions for kinetic perturbations.

It is informative to quantify the differences in sheath quantity response between fluid and kinetic equilibria used as initial conditions. The following quantity can be used as a measure of that deviation

$$\delta = |y_{KK} - y_{FK}|/y_{KK}, \quad (5.5)$$

where  $y$  is either  $\gamma_e$  or  $e\Delta\Phi/(kT_e)$ , while  $KK$  and  $FK$  denote values during the kinetic perturbation on the kinetic and fluid backgrounds, respectively. This quantity is plotted for several equilibrium input powers in Figure 5.13.

The fluid background cases underestimate both quantities (not shown here), and the “error” grows as input power is increased. The only exception is for  $\gamma_e$ , where the relative deviations seem to follow the rollover behaviour from Figure 5.7 and drop after  $3\text{MW}/\text{m}^2$ . For both sheath quantities,  $\delta$  is largest in the first  $\approx 2\mu\text{s}$  of the perturbation, with the  $\gamma_e$  deviation having secondary peaks after  $\approx 4\mu\text{s}$ . Values of  $\delta$  corresponding to peak value perturbations (around  $7-10\mu\text{s}$ ) of  $\gamma_e$  and  $e\Delta\Phi/(kT_e)$  are below 25% and 5%, respectively. The best agreement between

the fluid and kinetic backgrounds is for the lowest input power, so the  $\gamma_e$  peak value error for the  $1\text{MW}/m^2$  input power is indeed lowest - at less than 5%. The greatest  $\gamma_e$  error, however, is observed for the input power of  $3\text{MW}/m^2$ . This input power corresponds to both the peak equilibrium value of  $\gamma_e$ , as well as an equilibrium that is detached for kinetic and attached for fluid electrons. As such, it is to be expected that two qualitatively different equilibria would produce the greatest difference in quantitative perturbation responses.

## 5.4 Discussion

**Equilibrium kinetic effects:** In equilibria, kinetic effects are present but not dominant. Spatially dependent heat flux enhancement and suppression are observed, as shown in Figure 5.3, leading to steeper temperature gradients (see Figure 5.2), as well as detachment at higher input powers. The spatial and input power dependence on heat flux behaviour makes it difficult, if not impossible, to prescribe a heat flux limiter that would capture the observed kinetic behaviour. This is further emphasised in the comparison with the Two-Point Model, where the effective heat conductivity observed depends on the input power (Figure 5.4). The sheath heat flux coefficient exhibits rollover-like behaviour, peaking at around 40% above the classical value of  $\gamma_e \approx 5$ , as shown in Figure 5.7. Since the usual approach in the literature when it comes to parameter scans is that of scans in collisionality, it is informative to approach the results of this study from the perspective of collisionality. To that end, Figure 5.14 shows the  $\gamma_e$  results from Figure 5.7, plotted with respect to collisionality (as defined in equation (2.20)), and compared to several other results from the literature. The magenta triangle in Figure 5.14 represents the highly radiative case of KIPP simulations[5], where energy was removed from a JET-like  $\nu^* = 15$  case, mimicking radiative losses. A non-radiative result obtained by Kupfer et al.[121] using the Vlasov-Fokker-Planck code FPET is also shown as a comparison. Finally, the classical result[12] is given by the black dashed line, and can be taken to represent values obtained with the PIC code BIT1[80]. One immediately notices that a large discrepancy exists between the various results in the literature. Given that the KIPP result for the highly radiative case seems to agree well with the results from SOL-KiT, it is natural to assume that the sheath heat transmission

coefficient depends strongly on the underlying bulk plasma background. For example, the non-radiative BIT1[80] and KIPP[5] values for  $\gamma_e$  are lower than those reported in this study, and they do not seem to agree between themselves, with FPET results not agreeing with either. A detailed analysis would be required to pinpoint exact causes of discrepancy between existing codes and investigated scenarios, and is beyond the scope of this thesis. However, qualitative “roll-over” behaviour observed in BIT1 and KIPP is reproduced by SOL-KiT, with the highly radiative KIPP value of  $\gamma_e$  agreeing quantitatively well with the obtained SOL-KiT curve.

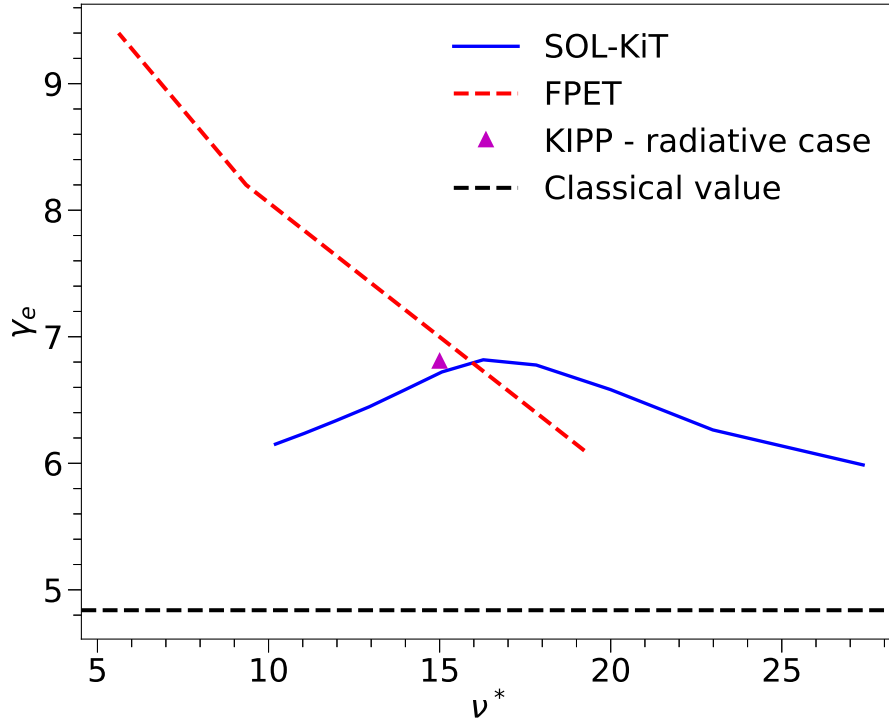


Figure 5.14: The sheath heat transmission coefficient plotted as a function of upstream collisionality  $\nu^*$ . SOL-KiT results are compared to results reported in the literature.

**Transient/perturbation runs:** Runs with transients, in contrast to equilibrium runs, appear to be affected much more by kinetic effects. Target temperature during kinetic simulations, as presented in Figures 5.8 and 5.9, is considerably lower compared with corresponding fluid runs. The heat flux behaviour is also strongly modified during transients. The ratio  $q/q_T$  varies both spatially and in time, as shown in Figure 5.10, with strong suppression and enhancement present throughout the perturbation. As such, there is very little hope that a fixed flux limiter would capture the observed behaviour. More complicated reduced non-local models (see, for example,

Brodrick et al.[119]) should be able to capture more than a simple flux limiter, and comparing them with the results obtained here would be an interesting study. The sheath heat transmission coefficient and the sheath potential drop are also found to be highly varying during the transient, as shown in Figure 5.12. As these two parameters act as boundary conditions in fluid codes, their strong variation further casts light on the flaws of fluid models in the context of SOL modelling. This result agrees with observations from BIT1 runs[80]. Note that all performed perturbation simulations were done in the same way, with only the initial conditions varying. It is found that kinetic effects are extremely sensitive to the initial conditions, i.e. the heating power of the utilised equilibrium. As noted above, this suggests that kinetic modification depends on the ratio of the energy content of the perturbation to that of the equilibrium. Further scans with varying equilibrium and perturbation powers would be required to investigate this. However, another avenue of exploration which can use the existing equilibria is the analysis of electron energy transport channels, and this will be presented in the next chapter.

#### 5.4.1 Limitations, computational cost, and further considerations

A number of assumptions and limitations are present in the model used, and it is worthwhile going over them. The first major assumption is that the problem is 1D. This does neglect cross-field transport and magnetic field effects, but for the sake of understanding parallel transport it should not be crucial. Furthermore, as both the fluid and kinetic model use the same assumptions, their comparison is still useful for revealing kinetic effects.

Two limitations of SOL-KiT are being tackled at the time of writing. These are the  $T_i = T_e$  approximation, as well as the limited neutral physics (currently only diffusive-reactive atoms included, with elastic electron-neutral collisions ignored). The consequence of these two limitations is primarily to restrict the accessible parameter space. However, the inclusion of molecules and impurities could help highlight further kinetic effects, as well as affect the general plasma background. This will be discussed in more detail in the following chapter.

While a number of possible optimisation steps can be taken to further speed up the computation of both equilibrium and transient simulations presented in this chapter, it is, nonetheless, worth commenting on current run times. All of the production runs analysed in this and the

following chapter were performed on single nodes (using 32 cores per node) through the Imperial College Research Computing Service[122]. Simulation times were not tracked directly, so the following numbers are all loose estimates, mainly based on requested job walltime. The fluid equilibrium runs took around 24h to complete ( $\approx 750\text{CPUh}$ ) per input power, while kinetic equilibria required employing the intrinsic coupling scheme (presented in Appendix E). Each kinetic simulation went through 6 iterations of the intrinsic coupling scheme ( $\approx 4500\text{CPUh}$ ) to remove acoustic transients, followed by a long kinetic relaxation (another  $\approx 5500\text{CPUh}$ ) to ensure that equilibrium is reached. It is very likely that both of these stages can be significantly optimised, especially if they are tailored to each individual input power. No such optimisation has been attempted during this study, as the intrinsic coupling scheme already reduces simulation times considerably compared to the brute force approach of completely kinetic runs. All transient simulations require less than  $\approx 750\text{CPUh}$  per full (heating and cooling) run. The computational time for the entire data set, based on the above (very) loose estimates, totals  $\approx 125\text{kCPUh}$ .

In this first study, the diffusive approximation ( $l_{max} = 1$ ) is used. While it can be expected that most of the physics is still captured, the approximation will naturally suppress kinetic effects, as the higher degrees of anisotropy are not accounted for. Since the heating operator is isotropic, the strongest driver of anisotropy will be the boundary condition, as the cut-off in the distribution function introduces strong anisotropy. However, preliminary results imply that higher harmonics tend to be localised near the boundary, and that a relatively small number of them is likely enough for satisfactory resolution of kinetic effects, as long as there is no strong driver of anisotropy in the sources.

Finally, the approach of launching kinetic perturbations on fluid equilibria is explored in Figures 5.8 and 5.13. It is found that, especially for lower power equilibria, this approach captures the qualitative perturbation behaviour well. Obtaining kinetic equilibria, even with coupling techniques, is computationally costly due to the need to resolve collisional timescales while equilibration occurs on much longer fluid scales. As such, the capability to run quick runs on fluid equilibria is a promising way to obtain qualitative results.

While current results are for MST conditions, qualitatively similar kinetic effects are likely

to manifest in larger machines for comparable collisionalities. Scaling of the simulation domain, particle density, as well as input power would allow moving into the parameter space of larger devices. An example would be simulations of JET, where the connection length is closer to  $L \approx 40m$ , upstream densities are of the order of  $10^{19}m^{-3}$ , which is about 2 times greater than the highest collisionality case examined here. This would, however, be computationally expensive due to the longer acoustic transition times, and most certainly require the use of coupling techniques to speed up convergence. This is another potentially exciting study the code would be capable of performing.

## 5.5 Summary

The results of a first equilibrium power scan and subsequent transient simulations performed on the obtained equilibria are presented in this chapter. Electrons are modelled as both a fluid and kinetically, and results of the different approaches are compared in order to identify kinetic effects and their consequences. The power scan was performed using medium size tokamak (MST) parameters, with input powers ranging from  $1MW/m^2$  to  $6MW/m^2$ . In this way, both attached and detached regimes are explored.

Kinetic effects have been noticed in both equilibria and transients, with them being dominant during perturbation simulations. Equilibrium kinetic effects include spatially dependent modification of the heat flux compared to classical values, as well as detachment onset at higher input powers compared to fluid simulations.

Sheath parameters (potential drop and heat transmission coefficient) change strongly during transient runs, leading to behaviour pure fluid codes cannot capture without resorting to questionable measures. Specifically, the sheath heat transmission coefficient varies up to 8 times its classical value during the perturbation, and the variation depends strongly on the initial energy content of the underlying equilibrium.

The limitations and possible extensions of the utilised approach are considered and discussed, with some of the next development steps outlined.

# Chapter 6

## Electron energy transport channel analysis

### 6.1 The energy equation and channels

As energy enters the SOL, assuming the simulation algorithm is conservative, it has to exit through one of several ways. These exit mechanisms will be referred to as channels. Since the transport of energy parallel to the magnetic field in the SOL is one of the determining factors for the divertor target heat load, understanding the channels through which it is transported is an important problem. This is especially true in the interaction of transients with detachment, as shifting energy from one channel to another can mean the difference between the target surviving or melting. In general, the number of energy transport channels can be quite high, owing to the many interactions the plasma can have with other species in the SOL. However, the number of channels in the simulations presented in the previous chapter is reduced due to model restrictions. These restrictions will be explored in more detail at the end of this chapter.

Taking the energy moment of the kinetic equation (3.1) produces the energy equation (more details in Appendix B)

$$\frac{\partial W_e}{\partial t} + \frac{\partial q_e}{\partial x} + eEn_e u_e = Q_{ext} + Q_{en}, \quad (6.1)$$

where  $W_e$  is the electron energy density. The inelastic energy transfer rate  $Q_{en}$  can be decomposed

into the radiated power density  $-Q_{rad}$  and the power density transferred to the neutrals through inelastic collisions  $-Q_n$ , where minus signs are introduced for convenience. If the energy equation is integrated over the entire domain, the following is obtained

$$\frac{\partial \int W_e dx}{\partial t} + q_{sh} + \int eEn_e u_e dx + \int Q_{rad} dx + \int Q_n dx = \int Q_{ext} dx, \quad (6.2)$$

where the fact that the upstream boundary is reflective is used, together with the knowledge that the outgoing heat flux is the sheath heat flux  $q_{sh}$ . In equilibrium this can be reduced to

$$q_{sh} + q_E + q_{rad} + q_n = q_{in}, \quad (6.3)$$

where the RHS represents the effective input energy flux, and the LHS the four major channels included in this study. The contributions of the four channels are expressed as effective energy fluxes, in units of power over (flux tube) cross-sectional area, which result from integrating individual power densities along the SOL. These channels are:

- The conductive and convective channel  $q_{sh}$  - delivered directly to the target by the electrons through the sheath,
- The electric field channel  $q_E$  - energy taken from the electrons by the electric field; transferred to the ions and delivered by them to the target,
- The hydrogenic radiation channel  $q_{rad}$  - energy radiated by the atomic neutrals; this is delivered to the target and the walls over a potentially larger area than the considered flux tube,
- The neutral transfer channel  $q_n$  - net energy transferred to the atoms via ionisation, and their inverse processes, used to maintain plasma density in equilibrium; this is delivered to the target by the ions and atoms as they impact it.

In order to explore the kinetic effects and general behaviour in the above channels, simulation results presented in the previous chapter will be revisited and looked at through the lens of

energy balance. For convenience, equilibrium temperature and density profiles for two different input powers are shown in Figure 6.1. Both the fluid and kinetic equilibrium results are plotted, with the choice of plotted input powers serving to illustrate further the fact that the different electron models detach at different points in the power scan. This will be explored in more detail quantitatively in the following section.

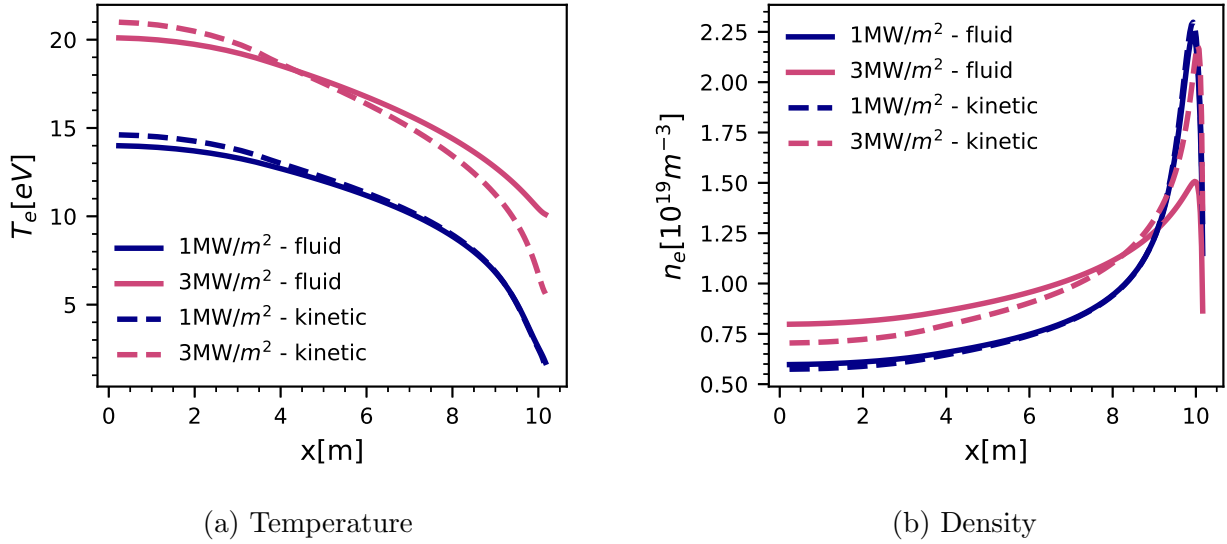


Figure 6.1: Temperature and density profiles for two different equilibria, simulated using both fluid and kinetic electrons. The intermediate input power of  $3\text{MW}/\text{m}^2$  is detached with kinetic electrons, and attached when electrons are treated as a fluid.

## 6.2 General channel behaviour

In equilibrium, as implied by (6.3), the considered channel contributions sum up to the input power flux, and the behaviour of the channels reflects the SOL regime. To illustrate how that behaviour changes, the various channel contributions are shown in Figure 6.2 as a function of input power for both fluid and kinetic electron modelling.

The different detachment onset behaviour discussed above and inferred from Figure 6.1 is also evident primarily from the radiation channels in Figure 6.2. Namely, Figure 6.2b shows a drop in radiated power at a higher input power when electrons are treated kinetically compared to the fluid case, indicating a presence of radiating neutrals, as well as a dense enough plasma to sustain radiation. A selection of percentage contributions to the four channels is given in Table

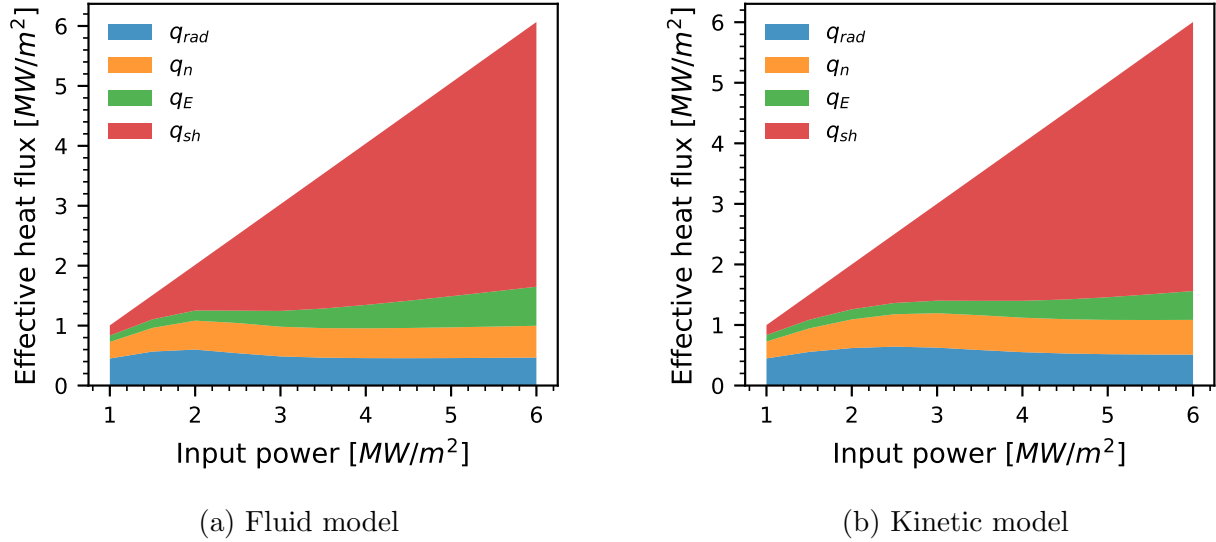


Figure 6.2: Contributions to the four channels in (6.3) when electrons are treated as a fluid or kinetically. The channels are: sheath heat flux ( $q_{sh}$ ), energy lost to electric field ( $q_E$ ), energy spent on maintaining ionisation and excitation states ( $q_n$ ), and energy lost to atoms that is subsequently radiated ( $q_{rad}$ ).

6.1 for three of the input powers, including  $3\text{MW}/\text{m}^2$ , at which, as noted, the kinetic runs are detached, while the fluid ones are not. Here, the radiated power difference between the fluid and kinetic models is quantitatively captured, as the percentage of input power radiated is 20.85% in the kinetic case, and 16.07% in the fluid case. One can also notice that the percentage power lost to the electric field  $q_E$  increases faster in the fluid case than in the kinetic runs. This is most likely the consequence of the electric field acting to balance higher pressure gradients near the boundary in hotter fluid runs, where the temperature increase also increases the pressure.

Table 6.1: Percentage contributions to the four channels in fluid/kinetic equilibria.

|             | $1\text{MW}/\text{m}^2$ | $3\text{MW}/\text{m}^2$ | $4.5\text{MW}/\text{m}^2$ |
|-------------|-------------------------|-------------------------|---------------------------|
| % $q_{rad}$ | 44.93/44.83             | 16.07/20.85             | 10.04/11.76               |
| % $q_n$     | 27.64/27.94             | 16.35/18.93             | 11.10/12.58               |
| % $q_E$     | 10.55/10.74             | 8.73/6.90               | 9.99/7.23                 |
| % $q_{sh}$  | 16.99/16.48             | 58.84/53.31             | 68.87/68.44               |

Based on the above results, kinetic effects on energy transport channels can be said to affect equilibrium simulations. However, as noted in the analysis of the simulation data in the previous chapter, kinetic effects are not dominant in equilibria, but manifest themselves strongly during conductive transients. To illustrate this in energy channel terms, similar stacked area plots as

in Figure 6.2 are plotted for the case of conductive transients, but with the  $x$ -axis this time corresponding to the time since the start of the perturbation. In the case of transients, the  $\partial \int W_e dx / \partial t$  term in (6.2) is not zero, and is not represented in the figures. The total energy content of the plasma changes during the transient, and the stacked plots in the figures below show the outgoing power for each of the channels.

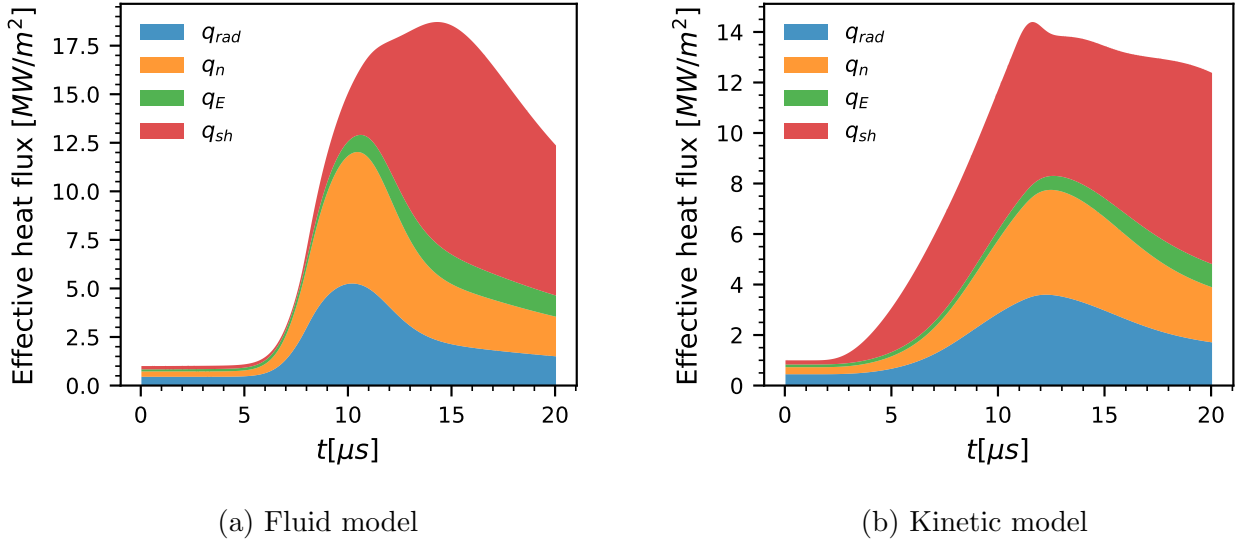


Figure 6.3: Effective outgoing energy flux associated with each channel during a  $45 \text{ MW}/\text{m}^2$  fluid perturbation on the  $1 \text{ MW}/\text{m}^2$  equilibrium. Note that the input power is reverted back to  $1 \text{ MW}/\text{m}^2$  after  $\approx 10 \mu\text{s}$ .

Figure 6.3 shows a comparison between the fluid and kinetic electron treatment of transients on the low power, detached equilibrium. Several points of difference are evident from the plotted energy channel contributions. Firstly, the peak outgoing power in the fluid electron case is greater than that in the kinetic case. Conversely, the kinetic channels appear to relax slower, especially throughout the relaxation phase, i.e. the second  $\approx 10 \mu\text{s}$ . This is likely due to upstream flux suppression, reducing the rate at which the perturbation energy is dissipated when kinetic effects are included. As noted in the previous chapter when looking at the target temperature in Figure 5.9, preheat is observed in the kinetic simulations. The same effect is visible in Figure 6.3b, where an initial increase in the sheath heat flux is present, yet it is not accompanied by an increase in radiation. This decoupling of the two channels can be explained by the fact that the fast particles reaching the divertor target after  $\approx 2.5 \mu\text{s}$  are too energetic to interact with the neutral cloud, and seem to ignore the detached front. In contrast to the

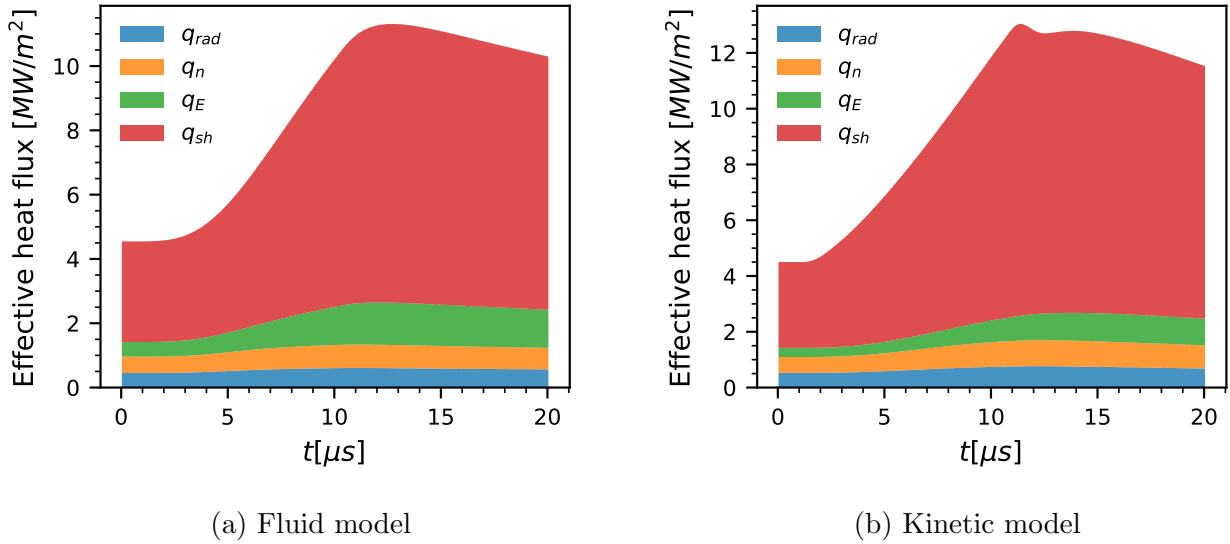


Figure 6.4: Effective outgoing energy flux associated with each channel during a  $45\text{MW}/m^2$  perturbation on the  $4.5\text{MW}/m^2$  equilibrium.

kinetic behaviour, in the fluid case in Figure 6.3a the increase in sheath heat flux is preceded by strong radiation and ionisation. The radiated power peaks also occur at different times for different electron models, with the kinetic peak occurring later and having a lower value. This reduced radiation is again a likely consequence of the heat flux suppression, and the resulting lower target temperatures. Lower target temperatures further lead to lower ionisation rates, and result finally in decreased detachment burn-through. However, kinetic effects in electron-atom interactions are also present, as will be discussed below.

On the other hand, the attached case with equilibrium input power of  $4.5\text{MW}/m^2$  does not show strong kinetic effects, as shown in Figure 6.4. While preheat is present, and the overall output power in the kinetic case is slightly higher, the fluid model appears to capture the energy dynamics well. As noted in the previous chapter, high power equilibria seem to be less susceptible to kinetic effects in general, likely due to an already flat profile and the fact that the tenfold power increase is not strong enough to produce gradients steep enough to generate significant non-local behaviour.

As noted above, the output power during transients is not equal to the instantaneous input power, as some of the input energy is retained in the plasma. If the simulations performed here were to be extended in time until a new equilibrium is reached, all of the perturbation energy

would have been evacuated through the various channels. Still, it is informative to look at the time-integrated channel fluxes for some of the perturbations, shown in Table 6.2. The first four rows of the table give integrated fluxes for each of the four channels for both the fluid and kinetic perturbations on equilibria already presented in Figure 6.2 and Table 6.1. The fifth row is just the total outgoing energy, i.e. the sum of the previous four rows. Finally, the last row represents the percentage of the input energy in the four channels, with the remaining input energy assumed to still be contained in the plasma. Several interesting observations can be made based on the data presented in Table 6.2, the first of which being that more energy appears to be delivered through the sheath channel during kinetic runs. This can be easily explained by the presence of preheat, as observed previously. Even with preheat, it would appear that the lowest power equilibrium experiences a slower energy exhaust overall. This is likely due to the fact that, in calculating the time-integrated fluxes, the phenomena of preheat and flux suppression act as competing processes. Further analysis with longer decay times is necessary to understand the full picture. However, the incompletely integrated fluxes currently available seem to support the observations reported in this chapter.

Table 6.2: Time-integrated fluxes (in units of  $J/m^2$ ) during **fluid**/**kinetic** perturbations on equilibria from Table 6.1. The last row shows the percentage of integrated input power that has left the electrons during the simulation time.

|                      | $1MW/m^2$     | $3MW/m^2$     | $4.5MW/m^2$   |
|----------------------|---------------|---------------|---------------|
| $w_{rad}$            | 41.89/38.28   | 13.59/20.04   | 11.09/13.41   |
| $w_n$                | 52.88/42.22   | 19.97/23.46   | 13.00/15.78   |
| $w_E$                | 15.70/5.93    | 16.83/9.47    | 19.58/12.43   |
| $w_{sh}$             | 93.57/86.00   | 112.90/150.90 | 129.17/153.81 |
| $w_{TOT}$            | 204.04/172.44 | 159.29/203.87 | 172.84/195.43 |
| $w_{TOT}/w_{in}[\%]$ | 44.26/37.40   | 33.11/42.38   | 34.84/39.39   |

### 6.3 Conductive and convective channels

The sheath heat flux channel contains two components, the conductive and convective heat fluxes. In order to better understand the heat flux leaving the system, it is useful to analyse the spatial profile of the heat flux and its components. In order to do that, the decomposition of the total electron heat flux throughout the simulation domain for two kinetic equilibria is shown in Figure 6.5. The chosen equilibria are again the representative attached and detached cases. The lower

power, detached equilibrium in Figure 6.5a shows a considerable convection contribution around the target, as would be expected in a detached regime due to the colder and denser plasma. The attached equilibrium (Figure 6.5b), however, shows a much greater conduction dominance up until very close to the target. The rapid increase in the convection contribution is due to the much narrower ionisation region caused by the narrow spatial profile of neutral density. In both cases, the uniform heating operator causes a spatial ramp up to the input power flux.

The main channel responsible for energy transport to the target during conductive transients is the sheath heat flux channel, as can be seen from the total area associated with it in Figures 6.3 and 6.4. To better understand the dynamics of this channel, its evolution is isolated in Figure 6.6. The kinetic effects discussed in the previous section become even more evident, with the preheat starting from  $\approx 2.5\mu s$ , and the kinetic perturbation showing a lower sheath heat flux peak in the detached case and a higher peak in the attached case. The  $1MW/m^2$  background experiences a slower decay and a second peak in the heat flux almost  $10\mu s$  after the heating is switched off. The slower decay of the kinetic perturbation is also evident on the  $1MW/m^2$  background. This further illustrates the heat load

“smearing” effect of flux suppression. It is interesting to note that, as can be seen from Table

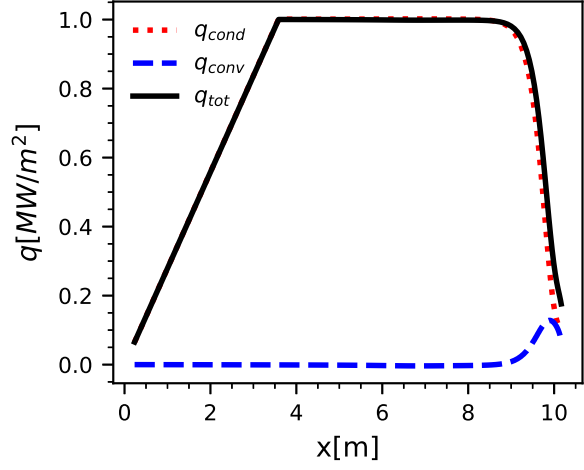
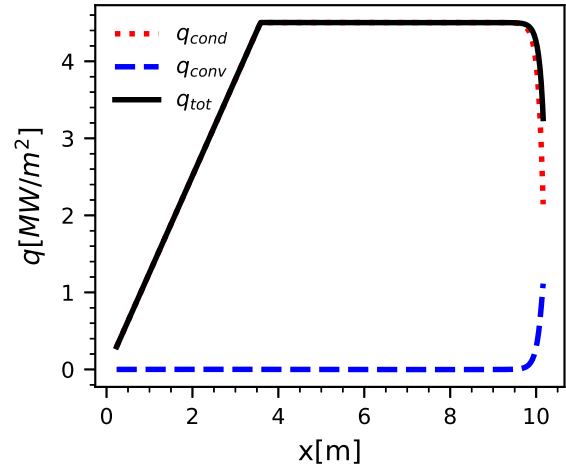

 (a)  $1MW/m^2$  equilibrium

 (b)  $4.5MW/m^2$  equilibrium

Figure 6.5: Conductive and convective electron heat fluxes in kinetic equilibria for detached and attached cases with input powers  $1MW/m^2$  and  $4.5MW/m^2$ , respectively. Negligible upstream convection contribution is a consequence of minor acoustic transients due to incomplete equilibration.

6.2, higher input power equilibria seem to allow a faster power loss through the sheath channel in the kinetic case. This could be due to the higher value of  $\gamma_e$  offsetting the effects of flux suppression.

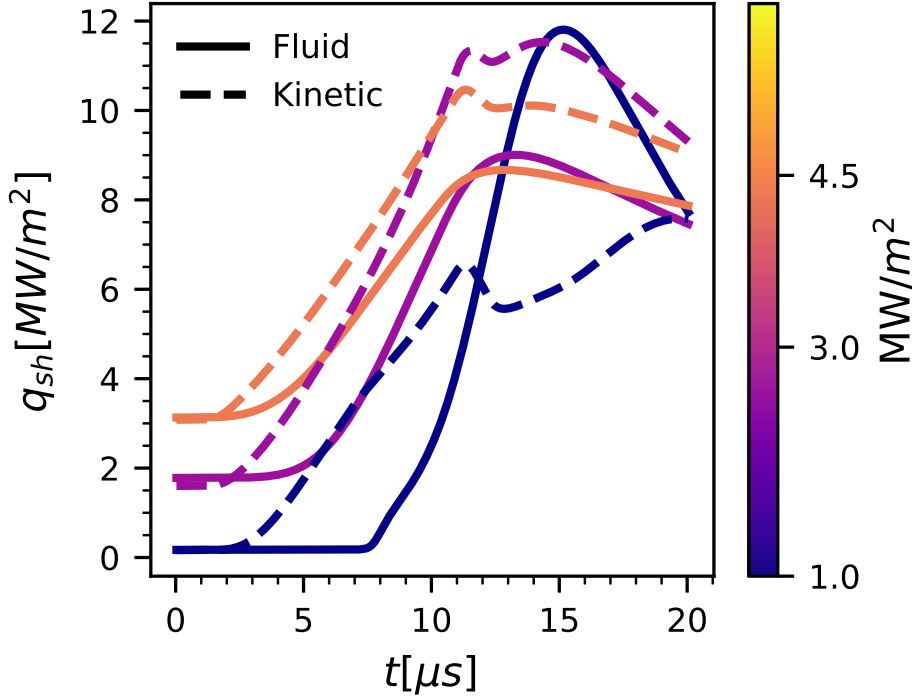


Figure 6.6: Evolution of the sheath heat flux channel corresponding to transients examined in the previous section.

## 6.4 The radiation and neutral transfer channels

The two channels involving electron interactions with atomic neutrals in the model are the radiation channel  $q_{rad}$  and the neutral transfer channel  $q_n$ . These channels can be further decomposed into their subchannels based on the particular radiative or collisional process they represent. The decomposition, in terms of the effective heat flux, can be written as

$$q_{rad} = q_{rad}^{deex} + q_{rad}^{recomb}, \quad q_n = q_{ex} + q_{ion} - q_{deex} - q_{recomb}, \quad (6.4)$$

where  $q_{rad}^{deex}$  and  $q_{rad}^{recomb}$  are the radiative deexcitation (line radiation) and radiative recombination (band radiation) contributions, while  $q_{ex}$ ,  $q_{ion}$ ,  $q_{deex}$ , and  $q_{recomb}$  are energy fluxes (power

densities integrated along the SOL) associated with the collisional processes of excitation, ionisation, deexcitation, and three-body recombination, respectively. To illustrate the subchannel decomposition, the power densities ( $\int W dx = q$ ) associated with each subchannel are plotted for the  $1\text{MW}/m^2$  kinetic equilibrium in Figure 6.7. As would be expected for an atomic hydrogenic plasma with temperature over  $1\text{eV}$ , recombination is weak, and the radiation channel is dominated by line radiation (magenta line in Figure 6.7). In most of the domain, the main contribution to the neutral transfer channel comes from ionisation and excitation. These two processes act to maintain the plasma density and the atomic state distribution in equilibrium. Near the target, however, superelastic collisions, in this case just collisional deexcitation, become non-negligible.

The fluid electron model decomposition of collisional-radiative power channels is not pictured here for the background in Figure 6.7. This is simply because the kinetic and fluid cases are nearly identical, supporting the finding by Zhao et al.[88] that kinetic effects on atomic rates in SOL equilibria are negligible.

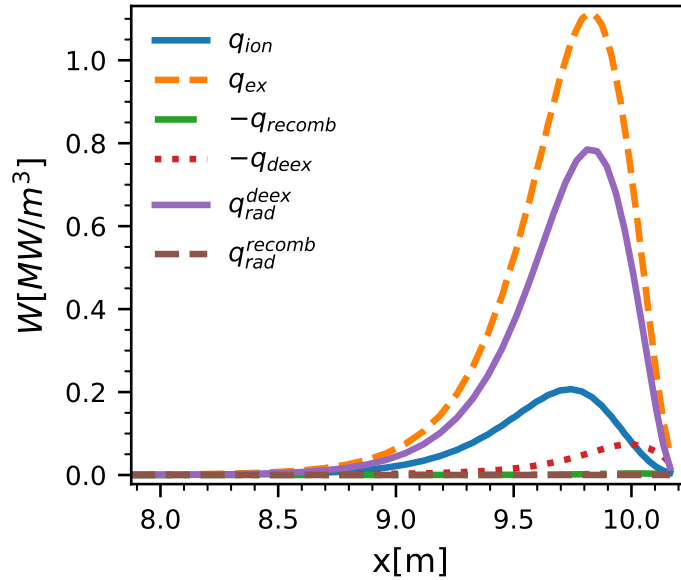


Figure 6.7: Various radiative and electron-neutral collisional subchannel contributions in the  $1\text{MW}/m^2$  kinetic equilibrium. These are: Ionisation  $q_{ion}$ , excitation  $q_{ex}$ , three-body recombination  $q_{recomb}$ , deexcitation  $q_{deex}$ , deexcitation radiation  $q_{rad}^{deex}$ , and recombination radiation  $q_{rad}^{recomb}$ .

In order to look at kinetic effects on inelastic collision rates during transients, the total

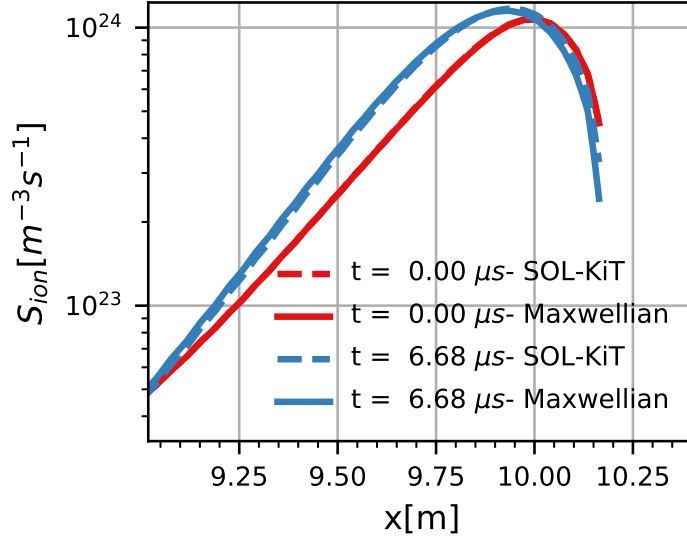
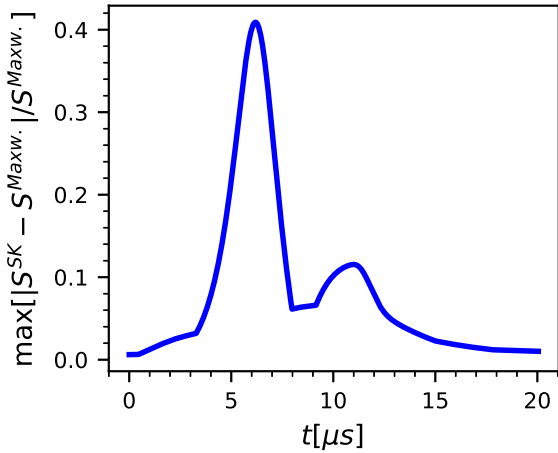
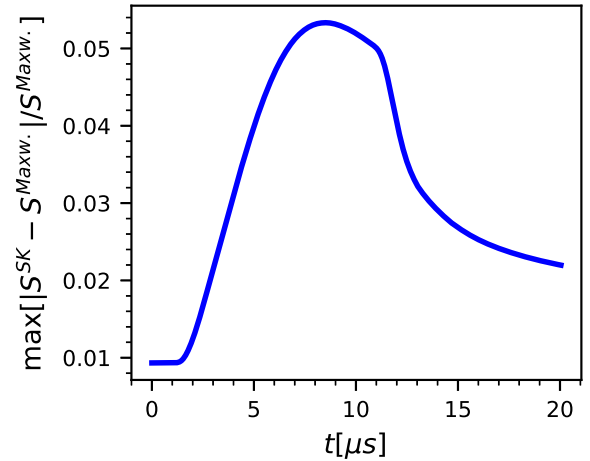


Figure 6.8: Ionisation sources at two times during the heating half of the conductive transient on the  $1\text{MW}/\text{m}^2$  background. The different lines represent ionisation sources calculated using the distribution obtained with SOL-KiT, as well as those calculated using a Maxwellian distribution with the same density and temperature as the SOL-KiT case.



(a)  $1\text{MW}/\text{m}^2$  background



(b)  $4.5\text{MW}/\text{m}^2$  background

Figure 6.9: Maximum relative deviation of ionisation source from that calculated by using a Maxwellian with same density and temperature for perturbations on the detached and attached equilibria.

ionisation source  $S_{ion}$  at the start and two thirds through the heating phase of the conductive transient on the  $1MW/m^2$  equilibrium is plotted in Figure 6.8. The figure shows a comparison between the sources calculated with the distribution obtained with SOL-KiT and sources that would result from a Maxwellian electron distribution with the same density and temperature. For an illustrative example of the evolution of  $f_0$  obtained with SOL-KiT close to the target the reader is referred to Figure 5.11, where the formation of a strong non-Maxwellian tail during the perturbation is visible. The overlapping lines at  $t = 0$  in Figure 6.8 indicate that the Maxwellian (fluid model) rates agree well with the kinetically obtained ones, as noted above. At  $t = 6.68\mu s$ , the rates calculated by SOL-KiT are different to those given by the fluid model. It is worth emphasising here that, in order to isolate kinetic effects on the rates, the plotted comparison is not one between a fluid and a kinetic perturbation. Instead, differing methods of rate calculation, based on different distribution functions, yet performed on the same macroscopic profile, are used to highlight kinetic effects. The distributions of atomic states used for both the SOL-KiT and Maxwellian ionisation source calculations are the same, further isolating the effect of rate modification to that of the differing electron distributions.

However, the logarithmic  $y$ -axis and the choice of plotted times in Figure 6.8, while enough to demonstrate a deviation from the fluid model, obfuscate the extent of the rate modification. In order to better grasp the evolution of rate modification and its extent, the maximum relative deviation of the ionisation source from fluid during the conductive transient is plotted in Figure 6.9 for both of the representative equilibria. The lower power equilibrium experiences ionisation source deviation reaching 40%, but quickly relaxes back toward lower values, while the attached case follows the general trend of kinetic effects being weaker for hotter equilibria, and the ionisation source does not deviate much more than 5% from the Maxwellian value.

Note that the ionisation rate results presented above indirectly include non-local effects on other atomic processes. For example, modifications of excitation rates factor in through multistep ionisation. In order to demonstrate that different processes can have very different non-local behaviour, the excitation rate for the  $2 \rightarrow 3$  transition obtained using SOL-KiT is compared to the equivalent Maxwellian rates in Figure 6.10. This particular process was chosen as it is one of the processes leading to the important Balmer alpha line emission used

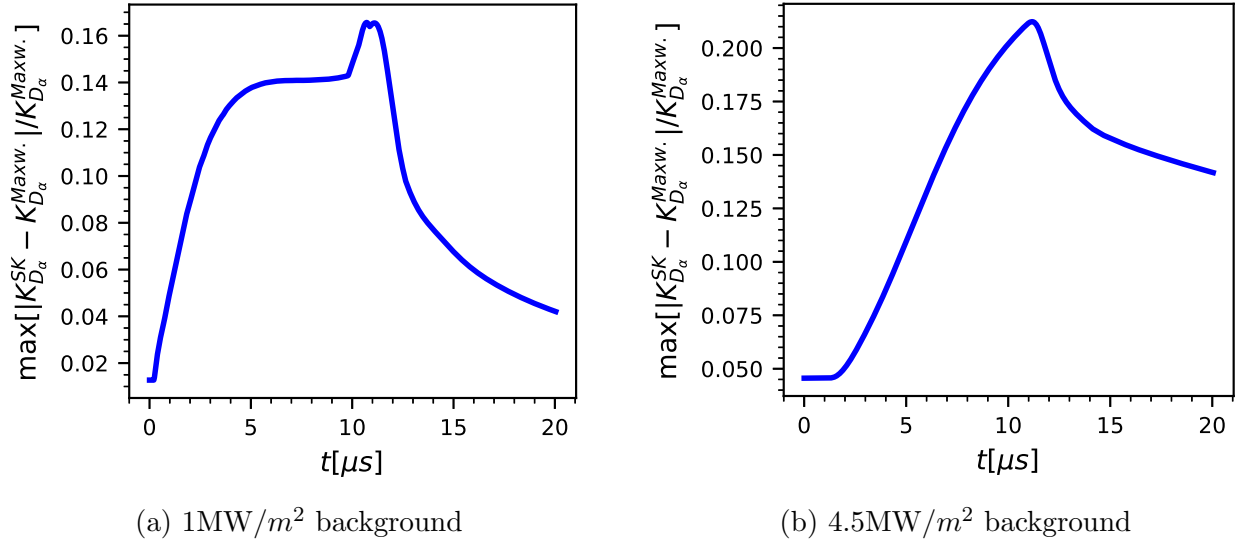
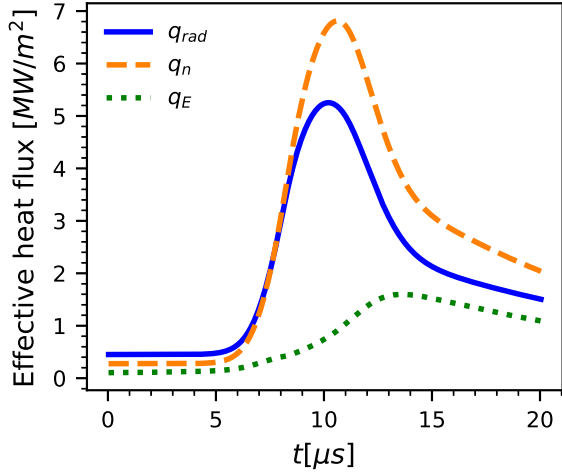
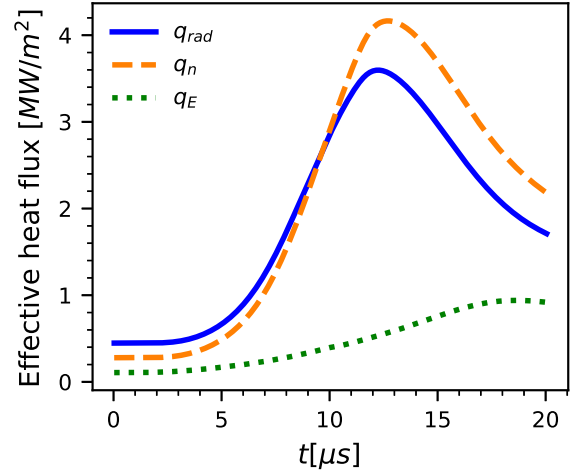


Figure 6.10: Maximum relative deviation of excitation rate for the  $2 \rightarrow 3$  transition calculated using the SOL-KiT distribution from rate calculated using an equivalent Maxwellian.

in ELM spectroscopic diagnostics. Specifically, it is the  $D_\alpha$  emission's direct collisional inverse process. What can be inferred from the deviation plotted in Figure 6.10 is that the behaviour is again very different for the lower and the higher power equilibrium. However, this time the higher power equilibrium shows a higher percentage deviation during the simulated conductive transient. This difference in behaviour is still compatible with the results shown in Figure 6.9, as the non-local effects in individual excitation processes do not necessarily have to all affect the final ionisation rate. In order to fully analyse the behaviour of each individual process, a post-processing solution capable of handling larger amounts of data is necessary. Such a framework has yet to be developed for SOL-KiT, and would have to include both data processing and improved output handling, as the number of tracked atomic processes is large. Nonetheless, even without necessarily tracking which (multistep) process is responsible for the ionisation deviation observed in Figure 6.9, kinetic effects on inelastic processes during transients have been demonstrated as both potentially important as well as complex.



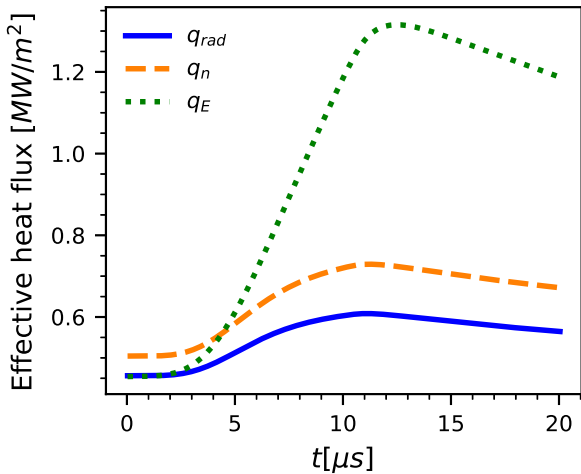
(a) Fluid perturbation



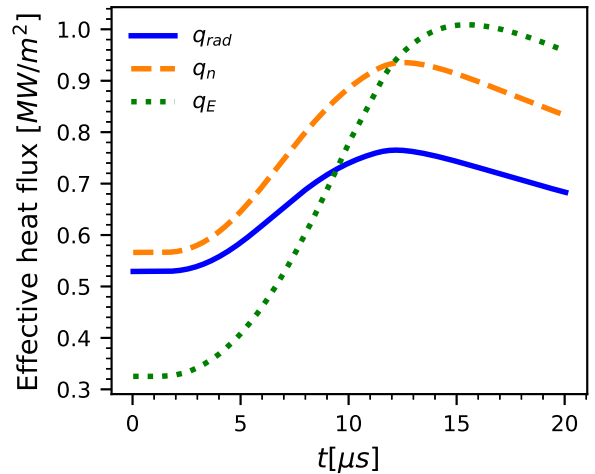
(b) Kinetic perturbation

 Figure 6.11: Evolution of the non-sheath channels during the perturbation launched on the  $1\text{MW}/\text{m}^2$  background, based on Figure 6.3.

For completeness and clarity, the evolution of the two neutral channels, as well as the electric field channel, during perturbations shown in stacked area plots in Figures 6.3 and 6.4 is presented in line plots in Figures 6.11 and 6.12. The differences between fluid and kinetic perturbations discussed in Section 6.2 can be seen here in a more quantitative manner, including both different peak values and positions of the different channel contributions.



(a) Fluid perturbation



(b) Kinetic perturbation

 Figure 6.12: Evolution of the non-sheath channels during the perturbation launched on the  $4.5\text{MW}/\text{m}^2$  background, based on Figure 6.4.

## 6.5 Discussion

**General and detachment behaviour:** Differences between channel contributions in fluid and kinetic equilibria are investigated in Figure 6.2, as well as in Tables 6.1 and 6.2. As noted in the previous chapter, it was found that detachment occurs at different input powers for different electron models. Namely, at an input power flux of  $3\text{MW}/\text{m}^2$ , the kinetic equilibrium is detached, and the fluid equilibrium is attached. In the energy channel analysis, this difference in detachment onset can be associated with the drop from  $\approx 21\%$  to  $\approx 16\%$  radiated power when moving from a kinetic to a fluid description. However, as previously found, kinetic effects become more striking in the case of conductive transients, when the input power flux is increased to  $45\text{MW}/\text{m}^2$  for  $\approx 10\mu\text{s}$ . Multiple effects have been observed during transients, and their intensity increases as the input power of the perturbed background is decreased, being most pronounced at the lowest power equilibrium considered. Preheat is evident in both low and high power cases, as shown in Figure 6.6, with hot electrons depositing energy through the sheath heat flux channel from  $\approx 2.5\mu\text{s}$ . Another interesting and potentially important effect that was observed was a spreading out of the sheath heat flux over a much longer period in the kinetic case compared to the fluid case, while its peak value was almost halved. The impact of this effect on divertor heat load and the dependence of the effect's strength on plasma regime require further research.

**Kinetic effects in electron-atom interactions:** By investigating the radiative and collisional channels, atomic rates were explored, and electron-neutral interactions were probed for kinetic effects. Research on kinetic effects in atomic rates for equilibrium SOL profiles was reported in the literature[88], and no significant modification of rates was found. The study performed in this work has confirmed the absence of kinetic effects in equilibria, but ionisation rates have been observed to vary significantly from their Maxwellian values during transient simulations. Figure 6.9a shows ionisation rates deviating up to 40% from those predicted by using a Maxwellian distribution during transients on a detached equilibrium. This effect is much weaker when the transient is launched on an attached background, however. While there is an increase in ionisation rates during kinetic transients launched on the  $1\text{MW}/\text{m}^2$  background

compared to equivalent Maxwellian rates, the overall ionisation rates are lower compared to fluid transient simulations, as can be inferred from the time integrated neutral transfer channel flux in Table 6.2. This leads to more of the detachment front surviving the transient, and the plasma not re-attaching when electrons are treated kinetically, as can be seen, for example, from the target temperature evolution in Figure 5.9. Previously, non-local effects on atomic rates during transients have been explored in the literature[3], but the simulated problem was a conductive relaxation of a ramp in temperature and ionisation degree, where a much stronger modification was observed. In order to observe similar strong modifications of hydrogenic ionisation rates it would likely be necessary to investigate either convective transients or use a power increase in input power in conductive transient simulations. More detailed power and density scans would be needed to investigate the maximum possible extent of non-local atomic effects in hydrogenic SOL plasmas.

### 6.5.1 Limitations

In this study, as was noted in the previous chapter, only the first two Legendre harmonics were used ( $l = 0, 1$ ). The effect of anisotropy on inelastic collisional processes depends on the anisotropy of the differential cross-section data used in the simulation. Accordingly, since all cross-sections are taken as integral cross sections with isotropic angular dependence, higher harmonics  $l > 0$  are dampened by collisions with neutrals. In reality, all inelastic collisional processes have some non-trivial angular dependence, which affects their interaction with higher harmonics. For example, the  $l = 1$  component of the differential cross-section determines the momentum-transfer rate of the particular inelastic process[123]. Similarly, elastic collisions of electrons with neutrals have a non-trivial angular dependence[124]. Unfortunately, to the author's knowledge, there is no systematic database of differential cross-sections for electron scattering on atomic hydrogen, elastic or otherwise. However, an interesting numerical experiment would be the introduction of an anisotropic differential cross-section, with several guesses for the angular dependence corresponding to forward/backward scattering, or some analytic form that would include multiple higher harmonics. While such a guessed form of the differential cross-section would not necessarily reflect reality, it would at least allow for the quantification of the effect of

added angular dependence in the scattering.

An important point about collisional processes is that they do not scale with machine size. Instead, they scale with density and temperature, meaning that associated length scales can stay relatively constant across different machines, especially in conduction limited and detached regimes, where temperatures near the target are relatively low. Firstly, this complicates the numerical treatment of larger machines, since approximately the same physical resolution needs to be used in order to resolve atomic processes of interest. Ignoring the increased computational cost associated with scaling up to larger machine sizes, the relatively constant nature of the inelastic mean free paths means that different connection lengths can have different effective collisionalities (expressed, for example, by the Knudsen number). However, it is the author's belief that, while exploring larger machines with SOL-KiT is definitely an area of interest, other physical effects, as discussed below, will have to be explored first in order to provide a large machine picture that is as realistic as possible.

A number of channels have been ignored in this study due to the approximations made in the SOL-KiT model. Firstly, electron-ion energy exchange has been ignored by setting  $T_i = T_e$ . As noted in the previous chapter's discussion, the effect of allowing the ion temperature to decouple from the electrons will likely be felt in higher power equilibria as well as during transients. Allowing the ion temperature to couple with the hot neutrals through charge-exchange would then provide further possible channels for energy transport, and it would be interesting to see the effects of the hot neutrals depositing their energy into the cold plasma near the divertor. Secondly, molecules and impurities are not yet included in the SOL-KiT model, and these would provide further radiation and neutral transfer channels. Other channels might include bremsstrahlung radiation, as well as effective cross-field transport. However, the comparison between fluid and kinetic modelling presented in this study, while limited in terms of energy channels, should still highlight kinetic effects well.

Finally, it should be noted that a likely place to find further electron kinetic effects in atomic processes in the SOL would be impurity ionisation and excitation rates. Impurities possess deeper potential wells, and thus collisional processes between electrons and these heavier atoms will have higher energy thresholds. This would lead to energetic tail electrons, those that have

ignored detachment in this study, being able to interact with impurities, manifesting non-local ionisation effects. At the time of writing, inclusion of impurity and molecular effects is a planned extension to SOL-KiT, and should hopefully lead to future insights in non-local atomic physics in the SOL.

### 6.5.2 Momentum loss and ionization cost

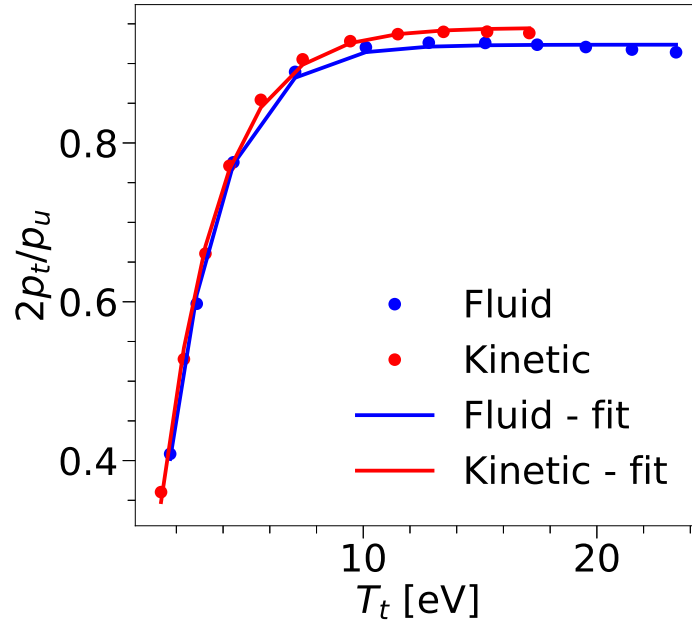


Figure 6.13: The pressure ratio plotted as a function of target temperature for both the kinetic and fluid equilibria, along with their respective fit functions.

**Momentum loss:** While an improved cross-section database would provide a better picture of momentum loss effects, which are key in obtaining detachment, it is still possible to characterise the obtained SOL-KiT results in this respect. The Two-Point Model without any momentum loss predicts  $2p_t = p_u$ , i.e. that the upstream pressure is twice the target pressure (as shown in Chapter 2). Accordingly, the following fit function is used in the literature to quantify momentum loss

$$\frac{2p_t}{p_u} = a \left[ 1 - \exp \left( \frac{-T_t}{b} \right) \right]^c, \quad (6.5)$$

where  $T_t$  is the temperature at the target. The pressure ratios obtained for each equilibrium run in both the fluid and the kinetic modes are plotted in Figure 6.13, alongside their fits using equation (6.5). Again, the lowest power equilibria agree well with each other, while the momentum loss seems to be slightly higher for the fluid model for greater input powers. This is likely due to lower momentum transfer rates when using a non-Maxwellian distribution function, but could also be due to other kinetic effects interacting in complex ways with the momentum loss mechanisms. A comparison between fit results obtained with SOL-KiT and several results from the literature is presented in Table 6.3. Both the fluid and the kinetic mode fit coefficients are comparable with other results, and seem to agree the most with SOLPS modelling of the ASDEX-Upgrade H-mode[45].

Table 6.3: Comparison of fit parameters from equation (6.5) obtained with the two SOL-KiT modes and those from the literature.

|                                      | <i>a</i> | <i>b</i> | <i>c</i> |
|--------------------------------------|----------|----------|----------|
| C-MOD experiments[125]               | 1.2      | 2.3      | 4.0      |
| ASDEX-U H-mode (SOLPS modelling)[45] | 0.8      | 2.0      | 1.2      |
| SD1D simulations[126]                | 0.9      | 2.1      | 2.9      |
| SOL-KiT - fluid                      | 0.9      | 2.0      | 1.5      |
| SOL-KiT - kinetic                    | 0.9      | 2.3      | 1.2      |

**Ionization cost and its role in detachment:** It is widely accepted in the field that detachment requires the presence of impurities. Traditionally, this has been carbon [127, 66, 128], but injected gas impurities are also used[44]. This naturally raises the question of how a detachment-like state is obtained using SOL-KiT and without any impurity radiation. In order to address this, it is worth repeating that the model presented here is 1D, with a limited neutral transport model, removing the potential deleterious effect of cross-field neutral transport. Furthermore, the line averaged densities treated in the presented study are on the low end when it comes to MST parameter space, likely contributing to a lower total energy content of the plasma. In order to obtain detachment-like behaviour it was necessary to perform a power scan, and similar behaviour is yet to be obtained in a density scan. However, similar modelling has been performed with a pure hydrogen plasma using the 1D fluid code SD1D[126], and detachment was observed with both a pure hydrogen plasma and one with a 1% carbon impurity content

during an upstream density scan. Interestingly, hydrogen radiation was found to dominate even in those runs with carbon present, demonstrating that, at least in a 1D simulation setting, impurities are not necessary to obtain detachment. The arguments extracted from the SD1D simulations point towards the combined importance of power and momentum loss in detachment onset. Specifically, it is argued that a rapidly decreasing ionisation cost (as a function of target temperature) is one of the key ingredients in reaching a detached state. The ionisation cost  $E_{iz}$  is defined as average energy removed from the electrons in atomic processes per ionisation, and can be calculated based on the following definition

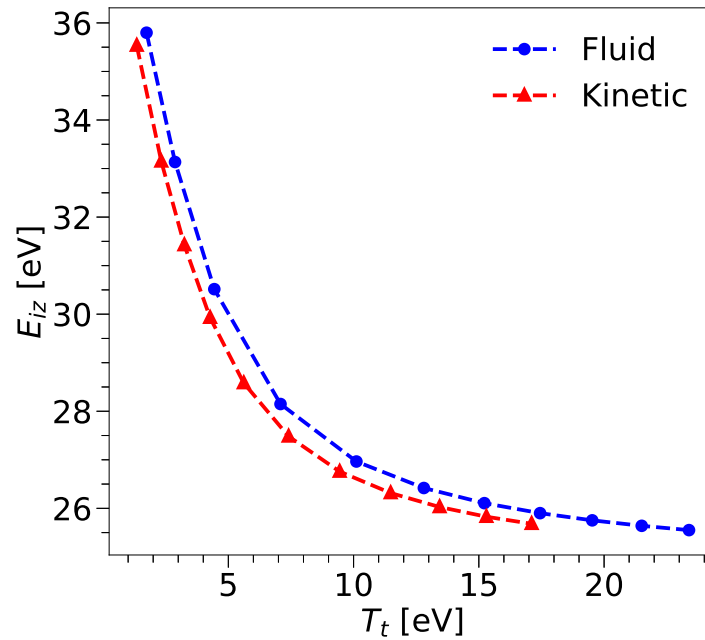


Figure 6.14: Effective ionisation cost plotted as a function of target temperature for both the kinetic and fluid equilibria.

$$q_n + q_{rad} = \Gamma_{sh} E_{iz}, \quad (6.6)$$

where it is assumed that the (effective) energy flux available for ionisation is that in the two neutral transfer channels. This definition assumes, of course, a steady state, and that no other channel contains energy that is potentially available for ionisation. Using the above definition, it is possible to determine the effective ionisation cost in SOL-KiT equilibrium runs, and this is plotted in Figure 6.14. The costs of ionisation are comparable between the fluid

and kinetic models, with the fluid model having a slightly higher cost. Again, this is likely due to the use of a Maxwellian distribution function for calculating the various rates, but could also be linked to other effects. Compared to SD1D results, however, the  $E_{iz}$  reported here is considerably lower, with SD1D results exceeding  $E_{iz} = 100eV$ . This could be due to a variety of reasons, but the most likely culprits are the use of different atomic databases and neutral models. However, the ionisation costs derived from SOL-KiT simulations are comparable to those obtained using spectroscopic methods on the TCV tokamak[129], where values in the approximate range  $17 - 50eV$  are reported.

## 6.6 Summary

The way energy is transported in the parallel direction of the SOL is important for determining the heat load on the divertor target, and consequently, the lifetime of the material. The different channels considered in this study are the sheath heat flux channel, the electron-neutral transfer channel, the radiative channel, and the electric field channel. These channel contributions are analysed in some detail in the above sections. The analysed simulation data is the same as the one presented in the previous chapter, and is comprised of fluid and kinetic equilibrium runs performed in a power scan, as well as runs with perturbations launched on the aforementioned equilibria.

A number of kinetic effects are observed in the channel behaviour presented in this chapter. Detachment offset effects noticed in the previous chapter have been further supported by the higher radiated power in kinetic equilibria. Furthermore, the domination of kinetic effects in transient simulations is again observed, this time in the form of preheat and atomic rate modification.

Limitations are discussed again, with a focus on missing energy channels and the potential refinement of existing channels. However, two important factors in detachment, momentum loss and ionization cost (effective energy cost per ionization event), have been compared with both experimental and theoretical investigations available in the literature, and satisfactory agreement, especially with experimental results, has been established.

# Chapter 7

## Conclusions

### 7.1 Summary of results

Understanding the physics determining divertor heat loads in MCF devices is crucial for the design of future reactors. Heat loads are strongly affected by various aspects of physics in the boundary region of these devices. Of special interest is the interaction of plasma perturbations with detachment, i.e. the neutral cloud protecting the divertor in a desirable high-collisionality regime. Both during transients/perturbations, as well as in equilibrium cases, one of the factors determining divertor heat load is parallel transport. Particles and energy are transported along magnetic field lines toward divertor targets, with various processes influencing the transport. Of those processes, collisions among plasma species as well as between the plasma and neutrals most strongly affect transport. Classic modelling of parallel transport relies on fluid models, often utilizing closures by Braginskii[18]. However, due to varying collisionality in the SOL, kinetic/non-local effects can become important, as the particle distribution functions start to strongly depart from Maxwellians.

In the study presented in this thesis, the focus was the understanding of kinetic effects in electron transport, in particular. The kinetic modelling of electron transport in the SOL required the development of a new code - SOL-KiT. Some of the special requirements set by the problem were the logical boundary condition and conservative electron-neutral collision operator differencing. Accordingly, the first formulation of the logical boundary condition in

terms of Legendre polynomials, as well as a novel conservative algorithm for inelastic collisions are present in SOL-KiT, and have been presented in detail in this thesis. SOL-KiT also allows for arbitrary Legendre harmonic expansion of the electron distribution, with an integrated capability of switching to a fluid model for the electrons. In this way, self-consistent comparisons are possible between the kinetic and fluid electron models, useful in highlighting kinetic effects. The SOL-KiT model, numerics, and various benchmarking tests are all presented, with special focus on the several novel aspects.

The novel capabilities of SOL-KiT have been partially exploited in a first study of SOL equilibria and transients. For equilibrium runs, a power scan was performed using parameters relevant to medium-size tokamaks. Equilibria were attainable due to the conservative nature of SOL-KiT algorithms, as well as a novel method of dynamically switching between the kinetic and fluid model for the electrons, speeding up convergence. Equilibrium kinetic effects include the modification of the heat flux, exhibiting both flux suppression and enhancement. This leads to kinetic equilibria being in general colder than the corresponding fluid equilibria. Steeper profiles produced by flux limiting contribute to lower target temperatures, effectively leading to detachment onset at higher input powers in the kinetic case than the fluid case. Non-monotonic behaviour is also observed in the sheath heat transmission coefficient, implying boundary condition behaviour in kinetic runs that is not present with electrons treated as a fluid. However, the main impact of kinetic effects was observed in simulations of conductive transients with the obtained equilibria used as backgrounds. Strongly time-dependent and spatially varying heat flux suppression and enhancement are both observed. Detachment is also found to be burnt through more slowly by the perturbation when electrons are treated kinetically. Finally, strong variations in boundary condition quantities, i.e. the sheath heat transmission coefficient, as well as the sheath potential drop, point toward the deficiency of boundary conditions in fluid models when used in time-dependent scenarios.

Relying on the energy conserving properties of SOL-KiT, an analysis of the various parallel electron energy channels and their behaviour was also performed. Different radiative channel behaviour supports the finding that detachment occurs at different points in the power scan for different electrons models. In investigating the sheath heat flux channel, preheat was observed,

pointing to energy being delivered by fast particles. Another effect that was found was the slower decay of the heat flux, likely caused by the upstream heat flux suppression. Kinetic effects on atomic rates were also investigated, with equilibrium effects being negligible, while significant non-local effects are observed during transient simulations.

## 7.2 Conclusions

Using self-consistent fluid comparison capabilities in SOL-KiT, kinetic effects could be isolated in both equilibrium and transient simulations performed in the presented study. Kinetic effects in equilibrium simulations can be considered present but not dominant. However, temperature profiles are steeper, detachment occurs at a higher input power, and the observed heat flux suppression and enhancement are likely not possible to mimic using fluid models with flux limiters. The sheath heat flux also exhibits non-local behaviour, varying up to  $\approx 40\%$  compared to the fluid model value, providing further difficulties in potential fluid modelling, as was noted in the literature by Havlíčková et al.[94].

Kinetic effects are dominant in the performed simulations of conductive transients, with kinetic simulations exhibiting very different behaviour to that observed with the fluid electron model. The most notable differences are in the perturbation behaviour on the low power, detached equilibria, where all of the kinetic effects observed were strongest. Firstly, target temperature and sheath heat flux are much lower in the kinetic perturbations with detachment. This leads, as noted above, to more resilient detachment fronts, potentially protecting the divertor better. However, due to energetic particles that form the preheat, as well as a longer decay time of the sheath heat flux, further investigation is required to understand the implications of the observed kinetic modifications on divertor heat load and material lifetimes. As for the sheath heat transmission coefficient, while it is modified in equilibria, its perturbation behaviour shows variation of almost a factor of 8 compared to its static classical value of  $\approx 5$ , consistent with the observation that kinetic effects are much stronger in time-dependent perturbation scenarios in the SOL.

The inelastic collision suite present in SOL-KiT allows the investigation of kinetic effects in

atomic rates. Confirming previous conclusions in the literature, equilibrium atomic rates appear to be well described by assuming a Maxwellian distribution for the electrons. In other words, no significant non-local effects were observed in the various atomic processes in equilibria. However, following the above trend of kinetic modifications becoming stronger when treating perturbations, ionisation rates are observed to change up  $\approx 40\%$  during transients, when compared to rates calculated using equivalent Maxwellian distributions. This effect is strongest when perturbations are launched on low power (detached) equilibria, becoming weaker as the background input power is increased. This general trend of kinetic effects being stronger on colder equilibria could also be interpreted in terms of detachment, and the resulting difference in electron energy between the upstream and downstream. In other words, a high input power but detached ITER or DEMO case could exhibit significant kinetic effects in conductive transients.

Considering the above results, the current study demonstrates the necessity of considering electron kinetic effects in simulations of the Scrape-Off Layer during transients, and, to a lesser extent, in particular equilibria. The non-trivial evolution of the boundary condition parameters during transients, as well as the spatially and temporally varying heat flux suppression and enhancement, pose a considerable problem to any attempt of fluid modelling. Looking at the wider implications of kinetic effects in transients, modifications to parallel temperature decay times could lead to different behaviour of L-mode filaments[17], coupling parallel and perpendicular transport, or in affecting detachment onset, as was observed in the results presented here. Thus, ignoring electron kinetic effects during (conductive) transients in models of the SOL/divertor potentially leads to both qualitative and quantitative errors.

A number of deficiencies with the utilized model and the performed simulations have been identified and discussed in detail. The capability of SOL-KiT to run with a higher number of Legendre harmonics has only been used for preliminary results at the time of writing, and refinement of the obtained results is an ongoing project. However, those preliminary results show that even the utilised diffusive approximation (simulating only harmonics up to and including  $l = 1$ ) captures the general behaviour well, while slightly underestimating kinetic effects. A project to include in SOL-KiT improved ion dynamics (the ion temperature equation), as well as impurity and molecular physics, is underway. The kinetic effects observed with hydrogenic

atoms in this study are expected to be much stronger when treating impurities, due to the much higher energy thresholds for electron-impurity inelastic collisions. With a higher energy threshold, the presence of energetic tail electrons should be felt more readily in the modification of atomic rates.

Finally, the range of applicability of the research software developed for this study should allow for investigations in multiple directions. Even with the base version of the code, ignoring the ongoing improvements, a number of MCF studies are within reach. For example, with the newly developed intrinsic coupling scheme, density scans in the SOL are a potential candidate for simulation. Scaling up the kinetic simulation domain to simulate large devices, or investigating different perturbation profiles are both potential future uses of SOL-KiT. Another use for SOL-KiT would be as a coupled module for a more sophisticated fluid code, providing it with the kinetic transport coefficients in a similar way they are provided when using intrinsic coupling. It would be most interesting to see not only how the code fares in some of these applications, but also the physical insight on kinetic effects that might result.

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# Appendix A

## Collision integral derivations

### A.1 Deriving the Rosenbluth potentials

Consider a Coulomb collision of a test particle with a field particle, with initial relative velocity  $\vec{v}_{rel} = v_{rel}\vec{e}_z$ , treated in the COM frame. Let the impact parameter vector be given by  $\vec{b} = b\cos\phi\vec{e}_x + b\sin\phi\vec{e}_y$ , where  $\vec{e}_x$  and  $\vec{e}_y$  are unit vectors along the  $x$  and  $y$  axes, and  $\phi$  is the azimuthal angle, i.e. angle between  $\vec{b}$  and  $\vec{e}_x$ . After collision, the particle will be deflected by an angle  $\theta$  towards the impact parameter vector, with the relative velocity vector post-collision being  $v_{rel}\vec{e}_z\cos\theta + v_{rel}\sin\theta(\cos\phi\vec{e}_x + \sin\phi\vec{e}_y)$ . As the collision is elastic,  $v_{rel}$  stays constant. The relative velocity change vector for a single  $b$  and  $\phi$  value is then given as

$$\Delta\vec{v}_{rel}(b, \phi) = v_{rel}\vec{e}_z(\cos\theta - 1) + v_{rel}\sin\theta(\cos\phi\vec{e}_x + \sin\phi\vec{e}_y). \quad (\text{A.1})$$

The differential cross-section for some  $\vec{b}$  is given by  $d\sigma(b, \phi) = bdbd\phi$ , and as a particle moves with velocity  $v_{rel}$ , it will collide with  $f_F(\vec{v}_F)d\vec{v}_Fd\sigma(b, \phi)v_{rel}\Delta t$  field particles after some time  $\Delta t$ . In order to get the total velocity change vector after that time, one must average  $\Delta\vec{v}(b, \phi)$  over both  $b$  and  $\phi$ , as well as the field particle distribution, i.e.  $d\vec{v}_F$

$$\Delta\vec{v}_{rel} = v_{rel}\Delta t \int f_F(\vec{v}_F)d\vec{v}_F \int_0^{2\pi} d\phi \int_{b_{90^\circ}}^{\lambda_D} \Delta\vec{v}(b, \phi)bdb. \quad (\text{A.2})$$

Since the integration is only over small-angle collisions (see integration bounds in  $db$  integral),  $\theta$  can be taken to be small in equation (A.1). Then

$$\Delta \vec{v}_{rel} = v_{rel} \Delta t \int f_F(\vec{v}_F) d\vec{v}_F \int_0^{2\pi} d\phi \int_{b_{90^\circ}}^{\lambda_D} \left( -\frac{v_{rel}\theta^2}{2} \vec{e}_z + v_{rel}\theta(\cos\phi \vec{e}_x + \sin\phi \vec{e}_y) \right) b db, \quad (\text{A.3})$$

where the  $\vec{e}_x$  and  $\vec{e}_y$  components vanish after integrating over  $d\phi$ . Using the small angle version of (2.48) the following can be written

$$\Delta \vec{v}_{rel} = -v_{rel}^2 \pi \Delta t \int f_F(\vec{v}_F) d\vec{v}_F \int_{b_{90^\circ}}^{\lambda_D} \left( \frac{q_T q_F}{2\pi\epsilon_0 b \mu v_{rel}^2} \right)^2 b db \vec{e}_z, \quad (\text{A.4})$$

which after integration in  $b$  gives

$$\Delta \vec{v}_{rel} = -\Delta t \int f_F(\vec{v}_F) d\vec{v}_F \frac{q_T^2 q_F^2}{4\pi\epsilon_0^2 \mu^2 v_{rel}^2} \ln \Lambda \vec{e}_z. \quad (\text{A.5})$$

Changing back into the lab frame, the change in the velocity vector of the test particle suffering collisions is  $\Delta \vec{v}_T = \mu \Delta \vec{v}_{rel} / m_T$ , thus giving

$$\Delta \vec{v}_T = -\Delta t \int f_F(\vec{v}_F) d\vec{v}_F \frac{q_T^2 q_F^2 (\vec{v}_T - \vec{v}_F)}{4\pi\epsilon_0^2 \mu m_T |\vec{v}_T - \vec{v}_F|^3} \ln \Lambda. \quad (\text{A.6})$$

Using basic vector calculus, this can be recast into

$$\Delta \vec{v}_T = -\frac{q_T^2 q_F^2 \ln \Lambda}{2\pi\epsilon_0^2 \mu m_T} \Delta t \frac{\partial}{\partial \vec{v}_T} \int \frac{f_F(\vec{v}_F)}{|\vec{v}_T - \vec{v}_F|} d\vec{v}_F, \quad (\text{A.7})$$

where the Rosenbluth potential  $\mathcal{H}_F$  from equation (2.56) can be identified. In order to derive the second Rosenbluth potential equation (A.1) is used to calculate  $\Delta \vec{v}_{rel}(b, \phi) \Delta \vec{v}_{rel}(b, \phi)$ . In order to avoid cumbersome notation, averaging over  $\phi$  is immediately performed (dropping all terms linear in  $\cos\phi$  or  $\sin\phi$ , and it is assumed that  $\theta$  is small (keeping only terms of order  $\theta^2$ ), so that

$$\int_0^{2\pi} \Delta \vec{v}_{rel}(b, \phi) \Delta \vec{v}_{rel}(b, \phi) d\phi = v_{rel}^2 \theta^2 \pi (\vec{e}_x \vec{e}_x + \vec{e}_y \vec{e}_y). \quad (\text{A.8})$$

Following the same approach as in the derivation of equation (A.5)

$$\Delta \vec{v}_{rel} \Delta \vec{v}_{rel} = \Delta t \int f_F(\vec{v}_F) d\vec{v}_F \frac{q_T^2 q_F^2}{4\pi\epsilon_0^2 \mu^2 v_{rel}} (\vec{e}_x \vec{e}_x + \vec{e}_y \vec{e}_y) \ln \Lambda. \quad (\text{A.9})$$

Denoting the unit tensor as  $\mathbf{I}$ ,

$$\frac{\vec{e}_x \vec{e}_x + \vec{e}_y \vec{e}_y}{v_{rel}} = \frac{v_{rel}^2 \mathbf{I} - \vec{v}_{rel} \vec{v}_{rel}}{v_{rel}^3}, \quad (\text{A.10})$$

which can be written in a more compact form by noting that

$$\frac{\partial}{\partial \vec{v}_T} \frac{\partial v_{rel}}{\partial \vec{v}_T} = \frac{v_{rel}^2 \mathbf{I} - \vec{v}_{rel} \vec{v}_{rel}}{v_{rel}^3}. \quad (\text{A.11})$$

Putting everything together (remembering that  $\Delta \vec{v}_T \Delta \vec{v}_T = \mu^2 \Delta \vec{v}_{rel} \Delta \vec{v}_{rel} / m_T^2$ ) gives

$$\Delta \vec{v}_T \Delta \vec{v}_T = \frac{q_T^2 q_F^2 \ln \Lambda}{2\pi\epsilon_0^2 m_T^2} \Delta t \frac{\partial}{\partial \vec{v}_T} \frac{\partial}{\partial \vec{v}_T} \int f_F(\vec{v}_F) |\vec{v}_T - \vec{v}_F| d\vec{v}_F, \quad (\text{A.12})$$

where  $\mathcal{G}_F$  from equation (2.57) can be recognised. The derivation presented here is based on the approach by Bellan [37].

## A.2 Simple derivation of the Boltzmann collision integral

The pre-, and post-collision velocities using the centre of mass quantities are given by

$$\vec{v}_{cm} = \frac{m_1 \vec{v}_1 + m_2 \vec{v}_2}{m_1 + m_2} = \frac{m_1 \vec{v}_1' + m_2 \vec{v}_2'}{m_1 + m_2}, \quad (\text{A.13})$$

and

$$\vec{v}_{rel} = \vec{v}_1 - \vec{v}_2, \quad (\text{A.14})$$

$$\vec{v}_{rel}' = \vec{v}_1' - \vec{v}_2'. \quad (\text{A.15})$$

This gives

$$\vec{v}_1 = \vec{v}_{cm} - \frac{m_2}{m_1 + m_2} \vec{v}_{rel}, \quad \vec{v}_1' = \vec{v}_{cm} - \frac{m_2}{m_1 + m_2} \vec{v}_{rel}', \quad (\text{A.16})$$

$$\vec{v}_2 = \vec{v}_{cm} + \frac{m_1}{m_1 + m_2} \vec{v}_{rel}, \quad \vec{v}_2' = \vec{v}_{cm} + \frac{m_1}{m_1 + m_2} \vec{v}_{rel}'. \quad (\text{A.17})$$

Noting that energy is conserved gives  $v_{rel} = v_{rel}'$ . The first step is to count the number of collisions experienced by particles with index 1 in a phase space volume  $d\vec{r}d\vec{v}_1$  around  $(\vec{r}, \vec{v}_1)$  in some time  $dt$ . Neglecting correlation between particles (Boltzmann's molecular chaos assumption), it can be said that there are  $f_1(\vec{r}, \vec{v}_1, t)d\vec{r}d\vec{v}_1$  particles in this volume. Taking  $d\sigma(v_{rel}, \Omega)$  as the differential cross-section, note that it sweeps out a volume (as in the Rosenbluth potential derivation) of  $d\sigma(v_{rel}, \Omega)v_{rel}dt$ . The number of particles with index 2 it sweeps through is then  $f_2(\vec{r}, \vec{v}_2, t)d\sigma(v_{rel}, \Omega)v_{rel}d\vec{v}_2dt$ . Putting it all together, the number of collisions in the considered phase space volume is

$$f_1(\vec{r}, \vec{v}_1, t)f_2(\vec{r}, \vec{v}_2, t)d\sigma(v_{rel}, \Omega)v_{rel}d\vec{r}d\vec{v}_1d\vec{v}_2dt,$$

which is the loss term in the integrand of the Boltzmann collision operator, as it counts collisions that cause particles to leave the phase space volume being considered.

Consider now collisions where post-collision velocities would be within  $d\vec{v}_1d\vec{v}_2$  around  $(\vec{v}_1, \vec{v}_2)$ . In other words, these are those collisions where the final state ends up in the monitored phase space region. Luckily, in the case of elastic collisions, time symmetry allows simply reversing the collisions and writing

$$f_1(\vec{r}, \vec{v}_1', t)f_2(\vec{r}, \vec{v}_2', t)d\sigma(v_{rel}, \Omega)v_{rel}d\vec{r}d\vec{v}_1'd\vec{v}_2'dt,$$

for the number of these inverse collisions. Effectively, this is counting all those particles with velocities in intervals  $\vec{v}_1' + d\vec{v}_1'$  and  $\vec{v}_2' + d\vec{v}_2'$  whose collisions produce final velocities around  $\vec{v}_1$  and  $\vec{v}_2$ . This represents the gain term.

In case of elastic collisions, it can be shown that  $d\vec{v}_1'd\vec{v}_2' = d\vec{v}_1d\vec{v}_2$ . This is equivalent to

showing that the Jacobian

$$\frac{\partial(\vec{v}_1', \vec{v}_2')}{\partial(\vec{v}_1, \vec{v}_2)} = 1. \quad (\text{A.18})$$

To do this, expand the Jacobian using the chain rule

$$\frac{\partial(\vec{v}_1', \vec{v}_2')}{\partial(\vec{v}_1, \vec{v}_2)} = \frac{\partial(\vec{v}_1', \vec{v}_2')}{\partial(\vec{v}_{cm}, \vec{v}_{rel})} \frac{\partial(\vec{v}_{cm}, \vec{v}_{rel})}{\partial(\vec{v}_{cm}, \vec{v}_{rel})} \frac{\partial(\vec{v}_{cm}, \vec{v}_{rel})}{\partial(\vec{v}_1, \vec{v}_2)}, \quad (\text{A.19})$$

where moving from the coordinate system  $(\vec{v}_1, \vec{v}_2)$  to  $(\vec{v}_1', \vec{v}_2)'$  is represented as a composite transformation:

1. Moving from  $(\vec{v}_1, \vec{v}_2)$  to the centre of mass frame before the collision  $(\vec{v}_{cm}, \vec{v}_{rel})$
2. Rotating the relative velocity vector  $\vec{v}_{rel}$  until it becomes  $\vec{v}_{rel}'$ , thus entering the centre of mass frame after collision  $(\vec{v}_{cm}, \vec{v}_{rel}')$
3. Moving from the centre of mass frame after the collision  $(\vec{v}_{cm}, \vec{v}_{rel}')$  to the lab frame  $(\vec{v}_1', \vec{v}_2')$

It is easy to show that the Jacobians arising from the coordinate transformations to and from the centre of mass frame are always unity. As rotating the relative velocity vector is a unitary operation, the determinant of the Jacobian for this step is unity as well. Thus  $d\vec{v}_1' d\vec{v}_2' = d\vec{v}_1 d\vec{v}_2$ , and the total change in particle number (with index 1) in phase space volume  $d\vec{r} d\vec{v}_1$  around  $(\vec{r}, \vec{v}_1)$  due to collisions can be written as

$$df_1 d\vec{r} d\vec{v}_1 = d\vec{r} d\vec{v}_1 dt \int d\vec{v}_2 \int d\sigma(v_{rel}, \Omega) v_{rel} [f_1(\vec{v}_1') f_2(\vec{v}_2') - f_1(\vec{v}_1) f_2(\vec{v}_2)], \quad (\text{A.20})$$

where integration was performed over all possible velocities of particles with index 2, as well as all possible collisions (i.e. deflection angles/impact parameters), making sure to attribute the gain and loss terms. By dividing by phase space volume and  $dt$  the basic form of the Boltzmann collision integral (2.59) is obtained.

# Appendix B

## Derivation of the electron fluid model

In this appendix the electron fluid model used in SOL-KiT will be presented in detail. The closure will be taken from the NRL Plasma Formulary[47], based on the Braginskii/Spitzer-Härm[18, 46] results, as presented in section 3.2.

For the purpose of the moment-taking in the following section, the kinetic equation used is

$$\frac{\partial f_e}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f_e - \frac{e}{m_e} \vec{E} \cdot \nabla_{\vec{v}} f_e = C_{ee} + C_{ei} + C_{en} + C_{heating}, \quad (\text{B.1})$$

where the RHS operators are the electron-electron, electron-ion, electron-neutral collision operators, as well as the heating operator, respectively.

### B.1 Continuity equation

The continuity equation is simply the zeroth moment of equation (B.1). The LHS will produce the same terms as in equation (2.64). Since all operators other than the ionisation and recombination parts of  $C_{en} = C_{ex} + C_{ion} + C_{recomb}$  on the RHS conserve particle number, the resulting continuity equation is

$$\frac{\partial n_e}{\partial t} + \nabla_{\vec{r}} \cdot (n_e \vec{u}_e) = S_e, \quad (\text{B.2})$$

where  $S_e = \int (C_{ion} + C_{recomb}) d\vec{v}$ . Using the definitions of the rates from section 3.4, the source can be rewritten as

$$S_e = \sum_b [n_b K_b^{ion} - \alpha_b n_e^2 n_i - \beta_b n_e n_i]. \quad (\text{B.3})$$

## B.2 Momentum equation

Multiplying (B.1) by  $m_e \vec{v}$  and integrating will yield the LHS of (2.67) with friction terms on the RHS

$$\frac{\partial(n_e m_e \vec{u}_e)}{\partial t} + \nabla_{\vec{r}} \cdot (n_e m_e \vec{u}_e \vec{u}_e) + \nabla_{\vec{r}} \cdot \mathbf{P}_e + n_e e \vec{E} = \vec{R}_{ei} + \vec{R}_{en}, \quad (\text{B.4})$$

where the pressure tensor is again defined using the random component of the electron velocity  $\mathbf{P}_e = m_e \int \vec{w} \vec{w} f_e d\vec{v}$ , while the friction terms are simply

$$\vec{R}_{ei} = m_e \int C_{ei} \vec{v} f_e d\vec{v}, \quad \vec{R}_{en} = m_e \int C_{en} \vec{v} f_e d\vec{v}, \quad (\text{B.5})$$

and it can be shown using the Legendre polynomial orthogonality relation that only the  $l = 1$  component of the individual collision operators contributes to the friction. Hence terms of the form given in equation (3.52) are obtained. Focusing on the first two terms in (B.4) the continuity equation can be extracted

$$\begin{aligned} \frac{\partial(n_e m_e \vec{u}_e)}{\partial t} + \nabla_{\vec{r}} \cdot (n_e m_e \vec{u}_e \vec{u}_e) &= n_e m_e \frac{\partial \vec{u}_e}{\partial t} + n_e m_e \vec{u}_e \cdot \nabla_{\vec{r}} \vec{u}_e + m_e \vec{u}_e \frac{\partial n_e}{\partial t} + m_e \vec{u}_e \nabla_{\vec{r}} \cdot (n_e \vec{u}_e) \\ &= n_e m_e \frac{\partial \vec{u}_e}{\partial t} + n_e m_e \vec{u}_e \cdot \nabla_{\vec{r}} \vec{u}_e + m_e \vec{u}_e S_e, \end{aligned} \quad (\text{B.6})$$

and the momentum equation can be recast as an evolution equation for the flow speed

$$\frac{\partial \vec{u}_e}{\partial t} = -\vec{u}_e \cdot \nabla_{\vec{r}} \vec{u}_e - \frac{\vec{u}_e}{n_e} S_e - \frac{\nabla_{\vec{r}} \cdot \mathbf{P}_e}{m_e n_e} - \frac{e}{m_e} \vec{E} + \frac{\vec{R}_{ei} + \vec{R}_{en}}{n_e m_e}. \quad (\text{B.7})$$

Finally, the form in section 3.2 is obtained by reducing the above equation to 1D, and taking isotropic pressure  $\mathbf{P}_e = n_e k T_e \mathbf{I}$ .

### B.3 Energy/Temperature equation

The final equation is obtained by taking the energy moment of (B.1) (multiplying by  $m_e v^2/2$  and integrating). The collisionless case is frequently treated in the literature, so the focus here will be on the effects of friction and sources. The first term in (B.1) upon integration yields

$$\int \frac{m_e v^2}{2} \frac{\partial f_e}{\partial t} d\vec{v} = \frac{\partial}{\partial t} \left[ \frac{3}{2} n_e k T_e + \frac{m_e n_e u_e^2}{2} \right], \quad (\text{B.8})$$

where the bracketed quantity is the total electron energy, including both thermal and kinetic flow energy. In all of the derivations in this section the decomposition of velocity into the flow and random parts  $\vec{v} = \vec{u}_e + \vec{w}$  is utilised to calculate the thermal components of the moments. Assuming no viscosity and isotropic pressure the second term yields

$$\int \frac{m_e v^2}{2} \vec{v} \cdot \nabla_{\vec{r}} f_e d\vec{v} = \nabla_{\vec{r}} \cdot \left[ \frac{m_e n_e \vec{u}_e}{2} (u_e^2 + 5kT_e) + \vec{q} \right], \quad (\text{B.9})$$

where the conductive heat flux is defined as  $\vec{q} = \int m_e w^2 \vec{w} f_e d\vec{w}/2$ . Thus the energy flow has been separated into the convective and conductive heat fluxes. The conductive flux used is the one presented in section 3.2, based on the results of Braginskii, Spitzer-Härm[18, 46], and Epperlein et al.[96, 95]. The electric field contribution to the energy equation is simply Ohmic heating  $e\vec{E} \cdot n_e \vec{u}_e$ , while the energy terms on the RHS are the collisional and external terms  $Q = Q_{en} + Q_{ext}$  defined as

$$Q_{en} = \int \frac{m_e v^2}{2} C_{en} d\vec{v}, \quad Q_{ext} = \int \frac{m_e v^2}{2} C_{ext} d\vec{v}, \quad (\text{B.10})$$

where the energy sources have been introduced in 3.2. The energy equation then becomes

$$\frac{\partial}{\partial t} \left[ \frac{3}{2} n_e k T_e + \frac{m_e n_e u_e^2}{2} \right] + \nabla_{\vec{r}} \cdot \left[ \frac{m_e n_e \vec{u}_e}{2} \left( u_e^2 + \frac{5kT_e}{m_e} \right) + \vec{q} \right] + e\vec{E} \cdot n_e \vec{u}_e = Q. \quad (\text{B.11})$$

To extract the temperature evolution equation from equation (B.11) the previous two moment equations must be eliminated. The continuity equation is easily eliminated by considering the

first two terms of (B.11), in the same way it was eliminated from the momentum equation. This yields

$$\begin{aligned} & \frac{3}{2}n_e k \frac{\partial T_e}{\partial t} + \frac{m_e n_e}{2} \frac{\partial u_e^2}{\partial t} + k T_e \nabla_{\vec{r}} \cdot (n_e \vec{u}_e) + \frac{m_e n_e \vec{u}_e}{2} \cdot \nabla_{\vec{r}} u_e^2 \\ & + \frac{5n_e \vec{u}_e}{2} \cdot \nabla_{\vec{r}} T_e + S_e \left[ \frac{3}{2} k T_e + \frac{m_e u_e^2}{2} \right] + \nabla_{\vec{r}} \cdot \vec{q} + e \vec{E} n_e \vec{u}_e = Q. \end{aligned} \quad (\text{B.12})$$

A number of familiar terms are starting to show up, but one more elimination is necessary. Combining the second, fourth, and last LHS term reveals the flow velocity evolution equation

$$\frac{m_e n_e}{2} \frac{\partial u_e^2}{\partial t} + \frac{m_e n_e \vec{u}_e}{2} \cdot \nabla_{\vec{r}} u_e^2 + e \vec{E} n_e \vec{u}_e = \vec{u}_e \cdot \left[ -n_e \vec{u}_e S_e - \nabla_{\vec{r}} \cdot \mathbf{P}_e + \vec{R}_{ei} + \vec{R}_{en} \right]. \quad (\text{B.13})$$

Again taking the pressure to be isotropic, and after cleaning up, the following temperature evolution equation is obtained

$$\begin{aligned} & \frac{3}{2}n_e k \left[ \frac{\partial T_e}{\partial t} + \vec{u}_e \cdot \nabla_{\vec{r}} T_e \right] + n_e k T_e \nabla_{\vec{r}} \cdot \vec{u}_e + S_e \left[ \frac{3}{2} k T_e - \frac{m_e u_e^2}{2} \right] + \nabla_{\vec{r}} \cdot \vec{q} + \vec{u}_e \cdot (\vec{R}_{ei} + \vec{R}_{en}) = Q, \end{aligned} \quad (\text{B.14})$$

which is easily reduced to one dimension and recast into the form of equation (3.7). Different physical terms can now be easily recognised. The first term is the material derivative of temperature, while the second is pdV heating, since  $p = n_e k T_e$ . The energy inflow associated with sources is balanced by the third term, while the conductive contribution is given by the divergence of the heat flux. Finally, frictional heating and energy exchange with neutrals and external sources round out the temperature equation.

# Appendix C

## Legendre polynomials

The following are all equivalent definitions of the Legendre polynomials

$$(1 - x^2) \frac{d^2 P_l(x)}{dx^2} - 2x \frac{dP_l(x)}{dx} + l(l+1) P_l(x) = 0, \quad (\text{C.1})$$

$$(l+1)P_{l+1}(x) - (2l+1)xP_l(x) + lP_{l-1}(x) = 0, \quad P_0(x) = 1, \quad P_1(x) = x, \quad (\text{C.2})$$

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l. \quad (\text{C.3})$$

$P_l(x)$  satisfy the following orthogonality relation

$$\int_{-1}^1 P_n(x) P_m(x) dx = \frac{2}{2n+1} \delta_{mn}, \quad (\text{C.4})$$

where  $\delta_{mn}$  is the Kronecker delta, as well as the parity property  $P_l(-x) = (-1)^l P_l(x)$ . In deriving the logical boundary condition the following derivative property is used together with the above recurrence relation

$$(1 - x^2)P'_l(x) = -lxP_l(x) + lP_{l-1}(x) = (l+1)xP_l(x) - (l+1)P_{l+1}(x). \quad (\text{C.5})$$

# Appendix D

## Detailed discretisation of SOL-KiT equations

Detailed discretisation of all equations in the SOL-KiT model will be presented here. This appendix draws heavily from the normalisation, grid, and timestep notation introduced in Chapter 4, and will thus contain only the formal discretisation of each equation. However, before that, an expanded list of derived normalisation constants appearing in the equations will be given. All spatial and velocity space derivatives will be written in shorthand and will be based on those presented in Section 4.4.

In all of the discretised equations the subscript  $k$  will denote the relevant spatial cell,  $n$  the velocity cell, and the superscript  $i$  or  $i^*$  the timestep or lagged timestep.

### D.1 Expanded normalisation

In the section below a number of equations will have normalisation constants present. These are summarised here.

$$A_{ee}^0 = \Gamma_{ee}^0 n_0 t_0 / v_{th}^3 = 1 / (Z \ln \Lambda_{ei}(T_0, n_0)),$$

$$A_{ei}^0 = \Gamma_{ei}^0 n_0 t_0 / v_{th}^3 = Z / \ln \Lambda_{ei}(T_0, n_0),$$

$$A_{en}^0 = v_{th} n_0 \sigma_0 m_e t_0 / (A m_p + m_e),$$

$$\begin{aligned}
 A_{en-l}^0 &= v_{th} n_0 \sigma_0 t_0, \\
 A_{spont}^0 &= 10^8 s^{-1} t_0, \\
 A_{rad-recomb}^0 &= n_0 t_0 10^{-25} s^{-1} m^3, \\
 A_{3b-recomb}^0 &= A_{en-l}^0 n_0 \sqrt{h^2 / (2\pi m_e T_0 [J])^3}, \\
 A_{diff}^0 &= \sqrt{m_e / m_i} / (2 n_0 \sigma_0 v_{th} t_0), \\
 A_{EJ} &= t_0^2 e^2 n_0 / (\epsilon_0 m_e) = t_0^2 \omega_p^2, \\
 A_{heat}^0 &= 1 MW m^{-2} / (m_e n_0 v_{th}^3), \\
 A_R^0 &= -t_0 n_0 / T_0^{3/2},
 \end{aligned}$$

where  $A$  is the atomic mass of the reference ion,  $m_p$  is the proton mass, and  $\omega_p$  is the reference plasma frequency.

## D.2 Fluid models and CRM

The ion and electron continuity equations are normalised and discretised as

$$\left( \frac{\partial n_e}{\partial t} \right)^{i+1} (x_k) = S_i^{i+1}(x_k) - \frac{\partial (n_e^{i*} u_e^{i+1})}{\partial x} (x_k), \quad (D.1)$$

$$\left( \frac{\partial n_i}{\partial t} \right)^{i+1} (x_k) = S_i^{i+1}(x_k) - \frac{\partial (n_i^{i*} u_i^{i+1})}{\partial x} (x_k), \quad (D.2)$$

where the source term is given as

$$S_i^{i+1}(x_k) = \sum_b \left[ A_{en-l}^0 K_b^{ion, i*} n_b^{i+1} - (A_{3b-recomb}^0 \alpha_b^{i*} n_e^{i*} n_e^{i+1} n_i^{i*} + A_{rad-recomb}^0 \beta_b^{i*} n_e^{i+1} n_i^{i*}) \right], \quad (D.3)$$

with all RHS terms evaluated at  $x_k$ . The discretised ion momentum equation is

$$\begin{aligned} \frac{\partial u_i^{i+1}}{\partial t}(x_k) = & -u_i^{i*}(x_k) \frac{\partial u_i^{i+1}}{\partial x}(x_k) + \frac{Zm_e}{m_i} E^{i+1}(x_k) + \frac{R_{ie}^{i+1}(x_k) + R_{CX}^{i+1}(x_k)}{m_i n_i^{i*}(x_k)} \\ & - \frac{S_i^{i+1}(x_k)}{n_i^{i*}(x_k)}(x_k) u_i^{i*}(x_k) - \frac{m_e}{2m_i n_i^{i*}(x_k)} \frac{\partial(n_i^{i+1} T_i^{i*})}{\partial x}(x_k), \end{aligned} \quad (\text{D.4})$$

where the electron-ion friction is calculated as

$$R_{ie}^{i+1}(x_k) = \frac{4\pi}{3} m_e \sum_{n=1}^{N_v} v_n^3 \Delta v_n C_{ei}^{i+1} f_1(x_k, v_n) = -R_{ei}^{i+1}(x_k). \quad (\text{D.5})$$

The same procedure is repeated for the numerically lost momentum in e-e collisions ( $C_{ei} \rightarrow C_{ee}$ ), conserving total momentum. See below for the case of fluid electron friction. The charge exchange friction operator is discretised as

$$R_{CX}^{i+1}(x_k) = -A_{en-l}^0 n_i^{i*}(x_k) m_i u_i^{i+1}(x_k) |u_i|^{i*}(x_k) \sum_b n_b^{i*}(x_k) \sigma_{CX,b}. \quad (\text{D.6})$$

Similarly to the ion momentum equation, the electron momentum equation is discretised as

$$\begin{aligned} \left( \frac{\partial u_e}{\partial t} \right)^{i+1}(x_k) = & -u_e^{i*}(x_k) \frac{\partial u_e^{i+1}}{\partial x}(x_k) + E^{i+1}(x_k) + \frac{R_{ei}^{i+1}(x_k) + R_{en}^{i+1}(x_k)}{m_e n_e^{i*}(x_k)} \\ & - \frac{S_e^{i+1}(x_k)}{n_e^{i*}(x_k)}(x_k) u_e^{i*}(x_k) - \frac{1}{2n_e^{i*}(x_k)} \frac{\partial(n_e^{i+1} T_e^{i*})}{\partial x}(x_k). \end{aligned} \quad (\text{D.7})$$

When electrons are treated as a fluid, the friction is calculated as  $R_{ei}^{i+1}(x_k) = R_u^{i+1}(x_k) + R_T^{i+1}(x_k)$ , where

$$R_u^{i+1}(x_k) = -A_R \times 1.48 \times 10^{-12} m_e n_e^{i*}(x_k) \frac{\ln \Lambda_{ei}^i(x_k) n_e^{i*}(x_k)}{(T_e^{i*})^{3/2}(x_k)} (u_e^{i+1}(x_k) - u_i^{i+1}(x_k)),$$

$$R_T^{i+1}(x_k) = -\frac{0.71}{2} m_e n_e^{i*}(x_k) \frac{\partial T_e^{i+1}}{\partial x}(x_k).$$

The electron-neutral friction is calculated by utilizing terms of the form

$$R_{en}^{ion,i+1}(x_k) = A_{en-l}^0 m_e \sum_b \frac{4\pi}{3} \sum_{n=1}^{N_v} \left( \frac{\delta f_1}{\delta t} \right)_b^{ion,i+1} (x_k) v_n^3 \delta v_n, \quad (D.8)$$

where  $\left( \frac{\delta f_1}{\delta t} \right)_b^{ion,i+1}$  is calculated using (4.49), with the exception that the drifting Maxwellian  $f_1$  is calculated at  $i^*$ , while  $n_b$  is taken to be implicit. For elastic electron neutral collisions, a similar approach is taken, but using the discretised form of the elastic electron-neutral collision operator (see below).

$$\begin{aligned} \left( \frac{\partial T_e}{\partial t} \right)^{i+1}(x_k) = & -u_e^{i*}(x_k) \frac{\partial T_e^{i+1}}{\partial x}(x_k) + \frac{2}{3} \left[ \frac{Q^{i+1}(x_k)}{n_e^{i*}(x_k)} - T_e^{i*}(x_k) \frac{\partial u_e^{i+1}}{\partial x}(x_k) \right. \\ & - \frac{2}{n_e^{i*}(x_k)} \frac{\partial q_e^{i+1}}{\partial x}(x_k) - \frac{S_i^{i+1}(x_k)}{n_e^{i*}(x_k)} \left( \frac{3}{2} T_e^i(x_k) - u_e^{i*}(x_k)^2 \right) \\ & \left. - 2 \frac{u_e^{i*}(x_k) (R_{ei}^{i+1}(x_k) + R_{en}^{i+1}(x_k))}{m_e n_e^{i*}(x_k)} \right], \end{aligned} \quad (D.9)$$

where all derivatives other than the advection derivative are central differenced. The heat exchange term  $Q = Q_{ext} + Q_{en}$  is differenced in the following way, keeping in mind that  $Q_{en} = Q_{el} + Q_{inel}$

$$Q_{ext}^{i+1}(x_k) = \Theta(2N_h + 1 - k) \frac{2A_{heat}^0 W_h T^{i+1}(x_k)}{T^{i*}(x_k) L_h}, \quad (D.10)$$

$$Q_{el}^{i+1}(x_k) = -\sum_b \frac{8}{\sqrt{\pi}} A_{en}^0 n_e^{i*}(x_k) n_b^{i+1}(x_k) \sqrt{T_e^{i+1}(x_k)} \sigma_{el}^1 (T_e^{i*} - T_g), \quad (D.11)$$

$$Q_{inel}^{i+1}(x_k) = -A_{en-l}^0 \sum_{b,b'} K_{b \rightarrow b'}^{i*}(x_k) n_b^{i+1}(x_k) \epsilon_{b \rightarrow b'}, \quad (D.12)$$

where  $\Theta$  is the (discrete) Heaviside step function, and the sum over  $b$  and  $b'$  includes both bound

and free electron states, where, when  $b$  denotes a free (ionised) state,  $n_b = n_e$ . The CRM is discretised as

$$\begin{aligned}
 \left(\frac{\partial n_b}{\partial t}\right)^{i+1}(x_k) &= A_{diff}^0 \frac{\partial}{\partial x} \left( D_b^{i*} \frac{\partial n_b^{i+1}}{\partial x} \right) \\
 &+ \sum_{b' < b} [A_{en-l}^0 (K_{b' \rightarrow b}^e)^{i*} n_{b'}^{i+1} - A_{spont}^0 A_{b \rightarrow b'} n_b^{i+1} - A_{en-l}^0 (K_{b \rightarrow b'}^e)^{i*} n_b^{i+1}] \\
 &+ \sum_{b' > b} [A_{spont}^0 A_{b' \rightarrow b} n_{b'}^{i+1} - A_{en-l}^0 (K_{b \rightarrow b'}^e)^{i*} n_b^{i+1} - A_{en-l}^0 (K_{b \rightarrow b'}^e)^{i*} n_b^{i+1}] \\
 &- A_{en-l}^0 (K_b^{ion})^{i*} n_b^{i+1} + A_{3b-recomb}^0 \alpha_b^{i*} n_i^{i*} n_e^{i+1} + A_{rad-recomb}^0 \beta_b^{i*} n_e^{i+1} n_i^{i*},
 \end{aligned} \tag{D.13}$$

where all RHS terms are evaluated at  $x_k$ , and the diffusive derivative follows the discretisation presented in the previous section. The diffusion coefficient is given by

$$D_b^{i*} = \frac{v_{tn}}{2[(n_i^{i*} + n_1^{i*})\sigma_{el} + \sigma_{CX,b} n_i^{i*}]} \tag{D.14}$$

Finally, Ampère-Maxwell's law is discretised as

$$\left(\frac{\partial E}{\partial t}\right)^{i+1}(x_k) = -A_{EJ}(j_e^{i+1}(x_k) + Z n_i^{i*}(x_k) u_i^{i+1}(x_k)), \tag{D.15}$$

where in kinetic mode the electron current is given by its corresponding moment, as defined in Chapter 4, and in the fluid mode it is simply  $j_e^{i+1}(x_k) = n_e^{i*}(x_k) u_e^{i+1}(x_k)$ .

### D.3 Discretisation of the electron kinetic equation

**Vlasov terms:** The Vlasov terms in the kinetic equations for the  $l$  harmonic are discretised following Section 4.4, and are given as

$$A_l^{i+1}(x_k, v_n) = -\frac{l}{2l-1} v_n \frac{\partial f_{l-1}^{i+1}}{\partial x}(x_k, v_n) - \frac{\partial f_{l+1}^{i+1}}{\partial x}(x_k, v_n), \tag{D.16}$$

$$E_l^{i+1}(x_k, v_n) = E^{i+1}(x_k) \left[ \frac{l}{2l-1} G_{l-1}^{i*}(x_k, v_n) + \frac{l+1}{2l+3} H_{l+1}^{i*}(x_k, v_n) \right], \tag{D.17}$$

where

$$G_l^{i*}(x_k, v_n) = v_n^l \frac{v_{n+1/2}^{-l} f_l^{i*}(x_k, v_{n+1/2}) - v_{n-1/2}^{-l} f_l^{i*}(x_k, v_{n-1/2})}{\Delta v_n}, \quad (\text{D.18})$$

$$H_l^{i*}(x_k, v_n) = \frac{1}{v_n^{l+1}} \frac{v_{n+1/2}^{l+1} f_l^{i*}(x_k, v_{n+1/2}) - v_{n-1/2}^{l+1} f_l^{i*}(x_k, v_{n-1/2})}{\Delta v_n}. \quad (\text{D.19})$$

**Coulomb collision operators:** Following the general ideas presented in 4.5, the operators are discretised and normalised as follows.

The electron-electron collision operator for  $l = 0$  was discussed in detail in Chapter 4, and the discretisation is repeated here for completeness

$$\left( \frac{\partial f_0}{\partial t} \right)_{e-e}^{i+1}(x_k, v_n) = \frac{A_{ee}^0 \ln \Lambda_{ee}(T_e^i(x_k), n_e^i(x_k))}{v_n^2} \frac{F^{i+1}(x_k, v_{n+1/2}) - F^{i+1}(x_k, v_{n-1/2})}{\Delta v_n}, \quad (\text{D.20})$$

$$\begin{aligned} F^{i+1}(x_k, v_{n+1/2}) &= C^{i*}(x_k, v_{n+1/2}) f_0^{i+1}(x_k, v_{n+1/2}) \\ &\quad + D^{i*}(x_k, v_{n+1/2}) \frac{f_0^{i+1}(x_k, v_{n+1}) - f_0^{i+1}(x_k, v_n)}{v_{n+1} - v_n}, \end{aligned} \quad (\text{D.21})$$

$$\begin{aligned} f_0^{i+1}(x_k, v_{n+1/2}) &= (1 - \delta^{i*}(x_k, v_{n+1/2})) f_0^{i+1}(x_k, v_{n+1}) \\ &\quad + \delta^{i*}(x_k, v_{n+1/2}) f_0^{i+1}(x_k, v_n), \end{aligned} \quad (\text{D.22})$$

$$\delta^{i*}(x_k, v_{n+1/2}) = \frac{1}{W^{i*}(x_k, v_{n+1/2})} - \frac{1}{\exp[W^{i*}(x_k, v_{n+1/2})] - 1}, \quad (\text{D.23})$$

$$W^{i*}(x_k, v_{n+1/2}) = (v_{n+1} - v_n) \frac{C^{i*}(x_k, v_{n+1/2})}{D^{i*}(x_k, v_{n+1/2})}, \quad (\text{D.24})$$

$$C^{i*}(x_k, v_{n+1/2}) = 4\pi \sum_{l=1}^n f_0^{i*}(x_k, v_l) v_l^2 \Delta v_l, \quad (\text{D.25})$$

$$D^{i*}(x_k, v_{n+1/2}) = \frac{4\pi}{v_{n+1/2}^*} \sum_{l=1}^n v_l^2 \left[ \sum_{m=l}^{N_v-1} f_0^{i*}(x_k, v_{m+1/2}) v_{m+1/2} (v_{m+1} - v_m) \right] \Delta v_l. \quad (\text{D.26})$$

The electron-electron collision operator discretisation for  $l > 0$  is based on the tridiagonal

matrices (4.25) and (4.26), and is given by

$$\begin{aligned}
 \frac{1}{A_{ee}^0 \ln \Lambda_{ee}(T_e^i(x_k), n_e^i(x_k))} \left( \frac{\delta f_l}{\delta t} \right)_{e-e}^{i+1}(x_k, v_n) &= 8\pi f_0^{i*} f_l^{i+1} + \frac{I_2^{i*}[f_0] + J_{-1}^{i*}[f_0]}{3v_n} \frac{\partial^2 f_l^{i+1}}{\partial v^2} \\
 &+ \frac{-I_2^{i*}[f_0] + 2J_{-1}^{i*}[f_0] + 3I_0^{i*}[f_0]}{3v_n^2} \frac{\partial f_l^{i+1}}{\partial v} \\
 &- \frac{l(l+1)}{2} \times \frac{-I_2^{i*}[f_0] + 2J_{-1}^{i*}[f_0] + 3I_0^{i*}[f_0]}{3v_n^3} f_l^{i+1} \\
 &+ \frac{1}{2v_n} \frac{\partial^2 f_0^{i*}}{\partial v^2} [C_1 I_{l+2}^{i+1}[f_l] + C_1 J_{-l-1}^{i+1}[f_l] + C_2 I_l^{i+1}[f_l] + C_2 J_{1-l}^{i+1}[f_l]] \\
 &+ \frac{1}{v_n^2} \frac{\partial f_0^{i*}}{\partial v} [C_3 I_{l+2}^{i+1}[f_l] + C_4 J_{-l-1}^{i+1}[f_l] + C_5 I_l^{i+1}[f_l] + C_6 J_{1-l}^{i+1}[f_l]] ,
 \end{aligned} \tag{D.27}$$

where all RHS terms are evaluated at  $(x_k, v_n)$ . The electron-ion collision operator for  $l > 0$  and stationary ions is simply discretised as

$$\left( \frac{\delta f_l}{\delta t} \right)_{e-i}^{i+1}(x_k, v_n) = -\frac{l(l+1)}{2} \frac{A_{ei}^0 n_i^{i*}(x_k) \ln \Lambda_{ei}(T_e^i(x_k), n_e^i(x_k))}{v^3} f_l^{i+1}(x_k, v_n), \tag{D.28}$$

while the flowing ion discretisation relies on the integrals (4.27) and (4.28), and is given by

$$\begin{aligned}
 \frac{1}{A_{ei}^0 n_i \ln \Lambda_{ei}(T_e^i(x_k), n_e^i(x_k))} \left( \frac{\delta f_l}{\delta t} \right)_{e-i}^{i+1}(x_k, v_n) &= \frac{1}{v_n^2} I_0^{i*}[F_0] \frac{\partial f_l^{i+1}}{\partial v} + \frac{I_2^{i*}[F_0] + J_{-1}^{i*}[F_0]}{3v_n} \frac{\partial^2 f_l^{i+1}}{\partial v^2} \\
 &+ \frac{-I_2^{i*}[F_0] + 2J_{-1}^{i*}[F_0] + 3I_0^{i*}[F_0]}{3v_n^2} \frac{\partial f_l^{i+1}}{\partial v} \\
 &- \frac{l(l+1)}{2} \frac{-I_2^{i*}[F_0] + 2J_{-1}^{i*}[F_0] + 3I_0^{i*}[F_0]}{3v_n^3} f_l^{i+1} \\
 &+ \frac{1}{2v_n} \frac{\partial^2 f_0^{i*}}{\partial v^2} [C_1 I_{l+2}^{i+1}[F_l] + C_1 J_{-l-1}^{i+1}[F_l] + C_2 I_l^{i+1}[F_l] + C_2 J_{1-l}^{i+1}[F_l]] \\
 &+ \frac{1}{v_n^2} \frac{\partial f_0^{i*}}{\partial v} [C_3 I_{l+2}^{i+1}[F_l] + C_4 J_{-l-1}^{i+1}[F_l] + C_5 I_l^{i+1}[F_l] + C_6 J_{1-l}^{i+1}[F_l]] ,
 \end{aligned} \tag{D.29}$$

with the RHS again evaluated at  $(x_k, v_n)$  to lighten notation.

**Electron-neutral collision operators:** The elastic electron-neutral collision integrals are discretised following an approach similar to the Coulomb operators. For  $l = 0$ , this produces

$$\left(\frac{\partial f_0}{\partial v}\right)_{el-en,b}^{i+1}(x_k, v_n) = A_{en}^0 n_b^{i*}(x_k) \frac{1}{v_n^2} \frac{F^{i+1}(x_k, v_{n+1/2}) - F^{i+1}(x_k, v_{n-1/2})}{\Delta v}, \quad (\text{D.30})$$

with

$$\begin{aligned} F^{i+1}(x_k, v_{n+1/2}) &= C(v_{n+1/2}) f_0^{i+1}(x_k, v_{n+1/2}) \\ &+ D(v_{n+1/2}) \frac{f_0^{i+1}(x_k, v_{n+1}) - f_0^{i+1}(x_k, v_n)}{\Delta v}, \end{aligned} \quad (\text{D.31})$$

where now the drag and diffusion coefficients are constants, and  $f_0^{i+1}(x_k, v_{n+1/2})$  is computed as in the electric field advection term. The drag and diffusion coefficients are simply

$$C(v_{n+1/2}) = v_{n+1/2}^4 \left( (1 - a_n) \sigma_{el,b}^{(1)}(v_{n+1}) + a_n \sigma_{el,b}^{(1)}(v_n) \right), \quad (\text{D.32})$$

$$D(v_{n+1/2}) = v_{n+1/2}^3 \left( (1 - a_n) \sigma_{el,b}^{(1)}(v_{n+1}) + a_n \sigma_{el,b}^{(1)}(v_n) \right) \frac{T_g}{2}, \quad (\text{D.33})$$

where  $a_n = 1 - 0.5\Delta v_n/\Delta v_{n+1}$  is the linear interpolation constant for the velocity grid. The elastic electron-neutral collision operator for  $l > 0$  is trivially discretised as

$$\left(\frac{\partial f_l}{\partial t}\right)_{b,el-en}^{i+1}(x_k, v_n) = -A_{en-l}^0 n_b(x_k) v_n \sigma_{el,b}^{(1)}(v_n) f_l^{i+1}(x_k, v_n). \quad (\text{D.34})$$

For the inelastic collisions, the normalised version of equation (4.49) is

$$\begin{aligned} \left(\frac{\delta f_l}{\delta t}\right)_{b \rightarrow b'}^{inel,i+1}(x_k, v_n) &= -A_{en-l}^0 n_b^{i*}(x_k) [\sigma_{b \rightarrow b'}^{TOT}(v_n) f_l^{i+1}(x_k, v_n) \\ &- \sum_m \sum_p W_{nm}^p (\sigma_{b \rightarrow b'}^{TOT}(v_m) - \sigma_{b \rightarrow b'}^{(l)}(v_m)) f_l^{i+1}(x_k, v_m)]. \end{aligned} \quad (\text{D.35})$$

**Heating operator:** The heating operator acting on  $f_0$  is discretised using the standard diffusion type derivative in velocity space

$$\left(\frac{\partial f_0}{\partial t}\right)_{heating}^{i+1}(x_k, v_n) = \Theta(2N_h + 1 - k) A_{heat}^0 D^{i*}(x_k) \frac{1}{v_n^2} \frac{\partial}{\partial v} v^2 \frac{\partial f_0^{i+1}}{\partial v}(x_k, v_n), \quad (\text{D.36})$$

where

$$D^{i*}(x_k) = \frac{W_h}{n_e(x_k)L_h}. \quad (\text{D.37})$$

**Particle source operators:** The particle source operator for  $f_0$  and the corresponding particle source for ions are implemented as

$$\begin{aligned} \left(\frac{\partial f_0}{\partial t}\right)_{source}^{i+1}(x_k, v_n) &= \Theta(2N_s + 1 - k)F_R(x_k)^{i+1} \left(\frac{1}{\pi T_{source}^{i*}(x_k)}\right)^{3/2} e^{-v_n^2/T_{source}^{i*}(x_k)} \\ &\times \frac{4\pi}{n_e^{i*}(x_k)} \sum_m v_m^2 f_0^{i+1}(x_k, v_m) \Delta v_m, \end{aligned} \quad (\text{D.38})$$

$$\left(\frac{\partial n_i}{\partial t}\right)_{source}^{i+1}(x_k) = \frac{\sum_m \left(\frac{\partial f_0}{\partial t}\right)_{source}^{i+1}(x_k, v_m) v_m^2 \Delta v_m}{n_e^{i*}}, \quad (\text{D.39})$$

where  $N_s$  is the total number of upstream cells affected by the source operator.

# Appendix E

## Iterative intrinsic coupling scheme for SOL-KiT

When attempting to reach equilibrium in SOL-KiT's kinetic electron mode, long simulation times can severely delay results. This is felt most strongly in runs where the collision times needed to be resolved are much shorter than the fluid time scale on which the density evolves through the relaxation of acoustic transients. In order to mitigate long run times, the following scheme was developed:

1. SOL-KiT is run in kinetic mode for a sufficiently long time for transport coefficients to equilibrate
2. Transport coefficients are either directly transferred to the fluid mode or otherwise treated with multipliers
3. The code is run in fluid mode
4. Upon return to the kinetic mode, the distribution function is guessed in an attempt to mitigate transients due to switching while maintaining macroscopic profiles

In short, the important aspects of the intrinsic coupling scheme are the two switches between modes. These are examined in detail below.

## E.1 Kinetic to fluid switch

When switching from kinetic to fluid mode for the electrons, the goal is to keep the behaviour obtained by the more accurate kinetic model, while allowing the fluid mode to quickly calculate the evolution of the density profile. In principle, four types of transport quantities (for  $l_{max} = 1$ ) need to be given to the fluid mode to maintain kinetic behaviour. These are:

- The heat conductivity
- The electron-ion friction coefficient
- Various inelastic collision rates
- The electron-neutral friction

Each of the above can either be tackled by taking the full value of the quantity in question and giving it to the fluid mode, or by calculating multipliers to be used in the fluid equations. All multipliers have the form  $M_A = A_K/A_F$ , where  $A_K$  is a quantity obtained in the kinetic mode, and  $A_F$  is the value of that quantity that the fluid model would predict with the same profiles as those used to calculate  $A_K$ . The fluid mode then multiplies the evolving  $A_F$  with the corresponding multiplier  $M_A$ , mimicking kinetic effects. The drawback of the first approach is that the quantities are frozen in time during the fluid run. Using multipliers avoids that problem, but introduces potential problems with unphysically large multipliers. The approach utilised in SOL-KiT is a combination of the two with minor modification, designed primarily to speed up equilibrium calculation convergence.

**Heat conductivity:** Multipliers are used to allow heat flux in the fluid mode to evolve in time. In particular, after the kinetic step,  $q/q_T$  is calculated and treated as a multiplier, ignoring the  $q_u$  contribution to the fluid heat flux, where  $q_T$  and  $q_u$  are given by equations (3.8) and (3.9). As long as there is a temperature gradient, this multiplier will not have unphysically high values. The only situation arising in the presented studies where the multiplier approach does not work is the temperature uptick observed in Chapter 5. In this case, multipliers lead to an unstable system, as they change sign close to the target. While not the perfect solution, the way

this is avoided is by taking the last non-negative value for the multipliers before they change sign and using that in the region where they are negative, i.e. close to the target. The fluid simulation are then unable to reproduce the uptick at the target, but result in a temperature profile close enough to the correct equilibrium that the final kinetic run can easily converge.

**The electron-ion friction force:** Similarly to the above, the friction force is treated using multipliers, this time calculating  $R_{ei}/R_T$ , and ignoring  $R_u$ . Unlike the heat conductivity problem, there was no need to remove negative multipliers for the friction force, as they do not introduce instabilities.

**Inelastic collision rates:** Again using multipliers,  $K/K_M$  is calculated, where  $K_M$  is the inelastic rate calculated using a Maxwellian. This is applied to each individual process.

**Electron-neutral friction:** Unfortunately, multipliers for electron-neutral friction do not work, due to the appearance of unphysically large values. This is due to the fact that the fluid mode friction can be extremely small, as there are locations in the SOL where there is no flow velocity. As such, fixed friction terms must be implemented, which is accomplished by taking the local friction for each electron-neutral collisional process from the kinetic mode and normalizing it to the local neutral density  $R_{en}^b/n_b$ . This takes into account friction variation due to varying neutral density in the fluid mode, but due to the fixed nature of  $R_{en}$  it fails to capture electron density, temperature, and flow velocity variation. However, in practice there were no situations where such a flaw stopped the coupling algorithm from converging.

## E.2 Fluid to kinetic switch

While switching from the kinetic to the fluid mode amounts to a loss of information, as kinetic effects are condensed into simple multipliers or moments, switching back to the kinetic mode requires the reconstruction of the electron distribution function. Since the distribution function was not evolved during the fluid run, it is not possible to know what it would be. In other words, the distribution function must be guessed or approximated. In this section the approach

taken in reconstructing  $f_0$  and  $f_1$  is presented. The main concerns in such an attempt are the mitigation of any transients induced by switching (due to a guess being far off), and the preservation of the  $n$ ,  $T$ , and  $u$  profiles obtained in the fluid mode.

**Rescaling  $f_0$ :** The simplest choice for  $f_0$  would be a Maxwellian distribution. However, a Maxwellian might be far off the correct distribution, and a Maxwellian  $f_0$  might induce strong transients where there is a strongly non-local distribution. For this reason,  $f_0$  is rescaled in the following way.

Let  $f_0$ ,  $n$ ,  $T$ , and  $u$  be the electron  $l = 0$  harmonic, density, temperature, and flow velocity before the original switch from kinetic to fluid. Then  $E = nkT + m_e u^2/2$  is the total energy before the original switch. If  $f_0$  is rescaled so that its particle and energy moments are  $n'$  and  $E'$ , respectively, the new distribution function is

$$f'_0(v) = a f_0(bv), \quad (\text{E.1})$$

where the scaling coefficients are given by

$$b^2 = \frac{n'E}{nE'},$$

$$a = \frac{n'b^3}{n}.$$

Unfortunately, while the simple rescaling presented above works in the analytical case, it breaks down when considering a discrete grid, much in the same way as in the electron-neutral collision operator discretisation in Chapter 4. The solution is similar to that there, and the analytically calculated  $b$  is used to find two points on the grid  $m$  and  $m + 1$ , between which the analytical velocity  $vb$  lies. The numerical version of  $f'_0$  is then

$$f'_0(v_n) = c(df_0(v_{m_n}) + (1 - d)f_0(v_{m_n+1})), \quad (\text{E.2})$$

resulting in the following scaling conditions for the numerical parameters  $c$  and  $d$

$$4\pi \sum_n c(df_0(v_{m_n}) + (1-d)f_0(v_{m_n+1})v_n^2\Delta v_n = n', \quad (\text{E.3})$$

$$4\pi \sum_n c(df_0(v_{m_n}) + (1-d)f_0(v_{m_n+1})v_n^4\Delta v_n = E', \quad (\text{E.4})$$

which can be solved to obtain  $c$  and  $d$ . Some amount of care is necessary to avoid pathological situations where  $b = 1$ , when the simple rescaling  $f'_0(v) = af_0(v)$  should be applied.

Using the above method, it is possible to rescale  $f_0$  in such a way to both preserve the general character of the electron distribution function, as well as ensure the correct density and energy moments numerically obtained from the fluid run. In the equations presented here, the spatial indices were dropped to lighten notation, but the method works at any spatial location.

**Determining  $f_1$ :** It is tempting to attempt rescaling of  $f_1$ , but the rescaling quantities,  $u_e$  and  $q_{TOT}$ , are not always positive, causing difficulties in any rescaling attempt. Thus, the approach taken here starts with the assumption that  $f_1$  can be modelled by the simplified (normalised) kinetic equation

$$v \frac{\partial f_0}{\partial x} - E \frac{\partial f_0}{\partial v} = - - A \frac{n_i}{v^3} f_1 - B \frac{\partial f_0}{\partial v}, \quad (\text{E.5})$$

where the electron inertia term  $\partial f_1 / \partial t$  is ignored, and the RHS is in the form of the slow flow electron-ion collision operator (equation (3.40)). The two parameters,  $A$  and  $B$ , are obtained by taking the velocity and heat flux moments of the above equation. In discretised form, these equations are

$$An_e u_e + BD_1 = U, \quad (\text{E.6})$$

$$Aq_{TOT} + BD_2 = Q, \quad (\text{E.7})$$

where

$$U = \frac{4\pi}{3n_i} \left( \sum_n v_n^7 \Delta v_n \frac{\partial f_0}{\partial x}(v_n) - \sum_n v_n^6 \Delta v_n \frac{\partial f_0}{\partial v}(v_n) \right), \quad (\text{E.8})$$

$$Q = \frac{4\pi}{6n_i} \left( \sum_n v_n^9 \Delta v_n \frac{\partial f_0}{\partial x}(v_n) - \sum_n v_n^8 \Delta v_n \frac{\partial f_0}{\partial v}(v_n) \right), \quad (\text{E.9})$$

$$D_1 = \frac{4\pi}{3} \sum_n v_n^3 \Delta v_n \frac{\partial f_0}{\partial v}(v_n), \quad (\text{E.10})$$

$$D_2 = \frac{4\pi}{6} \sum_n v_n^5 \Delta v_n \frac{\partial f_0}{\partial v}(v_n). \quad (\text{E.11})$$

Using the above  $A$  and  $B$  are easily obtained. It is important to note that no partial integration was performed before discretizing the equations. In this way, the values of the moments of  $f_1$  are numerically set to  $n_e u_e$  and  $q_{TOT}$ .

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