MASTER

Design of a computational model for compressible, magnetized flows in Magnum PSI

Peerenboom, K.S.C.

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Design of a computational model for compressible, magnetized flows in Magnum PSI

Kim Peerenboom

Supervisors:
Prof. Dr. J.J.A.M. van der Mullen
Ir. M.J. van den Donker
Abstract

At the FOM Institute of Plasma Physics in Rijnhuizen, the Netherlands, the linear plasma generator Magnum PSI is under construction. The plasma generated by this device can be used for plasma surface interaction studies under conditions similar to those found in the divertor of a fusion reactor. Numerical studies can provide useful information both in the development and operation stage of Magnum PSI. For this reason, a design study is carried out to investigate the use of the plasma modeling platform Plasimo for numerical modeling of this plasma. Characteristic for the Magnum PSI plasma are the magnetic confinement of the plasma and the compressibility of the flow. The magnetic field introduces anisotropy in the transport of mass, momentum and energy. First steps are made in the implementation of this anisotropy in the fluid equations of Plasimo. Furthermore, the composition and flow calculation are critically investigated.
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Chapter 1

Introduction

1.1 Technology assessment

Warming of the climate system is unequivocal, as is now evident from observations of increases in global average air and ocean temperatures, widespread melting of snow and ice, and rising global average sea level [42].

Intergovernmental Panel on Climate Change

In her fourth assessment report [42], published in 2007, the Intergovernmental Panel on Climate Change (IPCC) states that global warming is undeniable. The consciousness that this warming can not be contributed to natural variations is rising. Together with the increasing concern of shortage of fossil fuels in the near future, climate changes have stimulated the search for alternative energy sources.

Nuclear fusion could possibly provide an alternative for fossil fuels. However, commercial fusion is not expected before 2050 [43], since many difficulties still have to be overcome. A step forward towards commercial fusion power is the building of the test fusion reactor ITER in Cadarache, France. The aim of ITER is to demonstrate the scientific and technical feasibility of fusion power. However, for ITER to become a success, the problem of finding a suitable material for the divertor has to be addressed.

The divertor is the part of the fusion reactor, where Helium and impurities are removed from the fusion plasma. This divertor is exposed to high fluxes of hydrogen ions and energy. Material research has to be carried out to find a material which can stand these harsh circumstances in the divertor. For
this reason, the Magnum PSI (Magnetized Plasma Generator and Numerical Modeling for Plasma Surface Interaction Studies) device will be built at the FOM Institute of Plasma Physics in Rijnhuizen, The Netherlands. Magnum PSI is planned to be finished at the end of 2009.

![Figure 1.1: Overview of Magnum PSI. Figure from [44].](image)

In figure 1.1 an overview of the Magnum PSI device can be seen. At the left side, hydrogen gas is fed into the plasma source. In the source, a current is drawn, which creates the plasma. The plasma is then accelerated and expands into the source chamber. From the source chamber, the plasma flows into the heating chamber, where the plasma is additionally heated. Both the source chamber and heating chamber are pumped by a vacuum system. The plasma beam is transported to the target at the right by a superconducting magnet, which confines the plasma in the radial direction.

Currently, Pilot PSI, the pilot version of Magnum PSI, is already in operation. In experiments with Pilot PSI, it has been shown that it is possible to produce ITER relevant ion and energy fluxes [17]. In Pilot PSI, however, material research in the so called 'strongly coupled regime' is not possible. In the strongly coupled regime, molecules and dust particles that come off the material surface are trapped in the plasma beam and remain part of the plasma-surface interaction system. To enter the strongly coupled regime, a larger plasma beam is needed than is present in Pilot PSI. With Magnum PSI, the strongly coupled regime should be achievable [24].
1.2 Modeling of Magnum PSI

The aim of Magnum PSI is to study plasma-surface interaction under the ITER like conditions of high ion flux density ($>10^{24} \text{m}^{-2} \text{s}^{-1}$) and high power density (10 MW/m$^2$) at relatively low temperatures ($<5$ eV). To determine whether these conditions are established, ion density, flow velocity and temperature of the plasma are key parameters. Numerical modeling is a useful tool to study these parameters in different settings. In this way, questions like: What is the influence of the neutral background gas on the supersonic plasma beam? and What is the influence of nozzle configuration on the ion flux density? can be answered. To be able to answer these questions with a numerical model, the model has to meet a number of requirements:

- **Flow** In the plasma source of Magnum PSI the plasma expands, forming a supersonic jet. The flow calculation thus has to be suitable for compressible flow and must be able to simulate shock waves. The strong magnetic field in Magnum PSI magnetizes the plasma. Due to this magnetization, transport coefficients become anisotropic. This anisotropy has to be taken into account in the viscosity.

- **Composition** The flow velocity in Magnum PSI is very high. Therefore, fluid dynamic time scales can exceed chemical kinetic time scales. If this is the case, the plasma is not in chemical equilibrium and transport and finite rate chemistry have to be taken into account. Due to the magnetic field, diffusion becomes anisotropic.

- **Temperature** Due to the magnetic field, heat conduction becomes anisotropic. This anisotropy has to be taken into account as well.

There have already been a number of simulations with different codes on different parts of Magnum PSI. Simulations of the expansion into the source chamber have, for example, been carried out with gas dynamics and MagnetoHydroDynamic (MHD) approaches [10]. The interaction of the plasma with the target is modeled with Molecular Dynamics (MD). The plasma in the heating chamber and around the target have been modeled with the B2-EIRENE code [2]. B2-EIRENE uses a fluid dynamic approach for the charged particles and a Monte Carlo solver for the neutrals. B2-EIRENE can give a detailed description of the plasma in front of the target, but is less suited for simulation of the plasma source and expansion of the plasma into the source chamber. In the future, it is intended that the plasma simulation platform Plasimo is going to be used for modeling of the source and the source chamber of Magnum PSI.
1.3 This report

This report discusses the application of the plasma modeling platform Plasimo for the modeling of Magnum PSI. It is examined how the requirements mentioned in 1.2 can be met in Plasimo. Chapter 2 gives an overview of the equations of Plasimo and describes the effect of the magnetic field on these equations. The main effect of the magnetic field will be the anisotropy in the transport coefficients. A simple approach of calculating these anisotropic coefficients is given in 3. For diffusion a more sophisticated approach is possible, which will be presented in chapter 4. The implementation of this anisotropic diffusion approach is validated in chapter 5. Chapter 6 explains the flow calculation of Plasimo and discusses changes to the flow code, which make compressible modeling possible. In chapter 7 the suitability of the Plasimo flow calculation for Magnum PSI is demonstrated by simulating shockwaves in supersonic jets. The composition calculation of Plasimo is discussed in chapter 8. Conclusions are given in chapter 9.
Chapter 2

Plasimo

2.1 Introduction

Plasimo (PLasma SImulation MOdel) is a modeling platform for numerical simulation of plasmas. Plasimo can deal with three types of transport modes:

1. Raytracing for radiation transport

2. Particle In Cell-Monte Carlo (PIC-MC) for the kinetic modeling of particles under low pressure conditions.

3. The continuum approach

This report is restricted to the continuum approach under steady state conditions. In the continuum approach, Plasimo solves fluid equations for mass, momentum and energy. These equations are discretized with the control volume method. A hybrid discretization scheme is used. For a more detailed description of Plasimo, see for example [13, 21].

In sections 2.2, 2.3 and 2.4 of this chapter, Plasimo’s fluid equations are presented. It is discussed how these equations will change under the influence of a magnetic field. Section 2.5 and section 2.6 discuss the closure of the set of equations and the iteration scheme, respectively.
2.2 The flow equations

When steady state is assumed, overall mass conservation for the plasma bulk can be written as:

$$\nabla \cdot (\rho \mathbf{u}) = 0,$$  \hspace{1cm} (2.1)

where $\rho$ is the mass density of the plasma and $\mathbf{u}$ the velocity of the plasma. The momentum balance for the plasma reads:

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau,$$  \hspace{1cm} (2.2)

with $p$ the pressure and $\tau$ the viscous stress tensor. When a magnetized plasma is modeled, the Lorentz force $\mathbf{j} \times \mathbf{B}$ should be added to the momentum balance, with $\mathbf{j}$ the current density and $\mathbf{B}$ the magnetic field. In a magnetic field, the viscosity coefficient becomes anisotropic. The calculation of this anisotropic viscosity coefficient is discussed in chapter 3. The solution procedure of the flow equations is explained in chapter 6.

2.3 The species balances

Plasmas in which the transport phenomena have much larger timescales than the species production and destruction terms are said to be in Local Thermodynamic Equilibrium (LTE). In an LTE plasma species densities can be obtained from the laws of equilibrium thermodynamics. Since flow velocities are rather large in Magnum PSI, LTE is not a good assumption and a non-Local Thermodynamic Equilibrium (nLTE) model must be used for the calculation of the species densities. In an nLTE model, balances are solved for each species in the plasma:

$$\nabla \cdot (n_i \mathbf{u}_i) = S_i,$$  \hspace{1cm} (2.3)

with $n_i$ the number density of species $i$, $\mathbf{u}_i$ the absolute velocity of species $i$ and $S_i$ the source term which describes the production and destruction of species in chemical reactions. The total velocity of a species can be separated in a convection and a diffusion velocity:

$$\mathbf{u}_i = \mathbf{u} + \mathbf{v}_i.$$  \hspace{1cm} (2.4)

The bulk velocity $\mathbf{u}$ follows from the flow calculation. In a magnetic field, diffusion becomes anisotropic. The calculation of diffusion in a magnetic field is discussed in chapter 3 and 4. The formulation of the species balance in terms of $n_i$, such as presented here, appears to give problems in the presence of temperature gradients. This is discussed in chapter 8.
2.4 The energy balances

When a nLTE model is used in Plasimo, two temperatures are calculated: the electron temperature $T_e$ and the heavy particle temperature $T_h$. The heavy particle energy balance is given by [5, 21]:

$$
\nabla \cdot \left( \sum_h C_h T_h \mathbf{u} \right) + \sum_h p_h \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q}_h = \tau_h : \nabla \mathbf{u} + Q_h, \tag{2.5}
$$

with $C_h$ the heat capacity of heavy particle species $h$. The partial pressure of species $h$ is given by $p_h$, the conductive heat flux by $\mathbf{q}_h$, the viscous stress tensor by $\tau_h$ and the energy change through elastic and inelastic processes by $Q_h$. The electron energy balance is given by [5, 21]:

$$
\nabla \cdot (C_e T_e \mathbf{u}) + p_e \nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q}_e = Q_{ohm} + Q_e, \tag{2.6}
$$

where $C_e$ is the heat capacity of the electrons, $Q_{ohm}$ the ohmic dissipation, and $Q_e$ the energy change through elastic and inelastic processes. Both the heavy particle and electron conductive heat flux become anisotropic in a magnetic field. Calculation of anisotropic heat conduction coefficients is discussed in chapter 3. As was already mentioned in 2.2, the viscous stress tensor becomes anisotropic as well.

2.5 Closure

In order to solve the set of equations presented in this chapter, the set must be closed. To this end, constitutive relations for the viscosity and heat conduction and an equation of state are used. In the standard calculation of transport coefficients in Plasimo, for the viscous stress tensor, a Newtonian fluid is assumed, where the dynamic viscosity is calculated according to [27]. Both for the electron and heavy particle heat flux, Fourier’s law is assumed, where the electron heat conductivity is calculated according to [15] and the heavy particle heat conductivity according to [27]. In chapter 3 it is discussed how these constitutive relations change under the influence of a magnetic field. The equation of state used in Plasimo is the ideal gas law:

$$
p = \sum_i n_i k T_i, \tag{2.7}
$$

which couples the hydrodynamic pressure to the species densities and temperature.
2.6 Iteration scheme

The equations presented in this chapter are iteratively solved using under-relaxation. The sequence of calculation of a nLTE model in Plasimo is as follows:

- Calculate the Ohmic dissipation $Q_{ohm}$
- Update the flow field (equations 2.1 and 2.2)
- Update the species densities (equation 2.3)
- Calculate the mass density $\rho$ from the species densities $n_i$
- Update the heavy particle temperature (equation 2.5)
- Update the electron temperature (equation 2.6)

The model is said to be converged when the residue is below a preset value (usually $10^{-8}$), where the residue $\xi$ is defined as:

$$\xi = \max_{i,j,N} \left| \frac{\Delta \Phi_{i,j}^N}{\Phi_{i,j}^N} \right|,$$

(2.8)

with $\Phi_{i,j}^N$ the solution of equation $N$ at gridpoint $(i, j)$. 
Chapter 3

A simple approach of anisotropic transport

3.1 Introduction

The behavior of a plasma is strongly affected by the presence of a magnetic field. Magnetic fields make the transport phenomena of the plasma direction dependent: they introduce anisotropy. Normally, without a magnetic field, particles in a plasma move randomly with their thermal velocity. Due to collisions, mass, momentum and energy of these particles is redistributed. In a magnetic field, charged particles spiral around the magnetic field lines. This spiraling motion causes the anisotropy in transport along, across and around the magnetic field lines. The motion of the particles across and around the field lines is coupled by the Lorentz force. This coupling causes so called diamagnetic fluxes.

In the first three sections of this chapter, diffusion, viscosity and heat conductivity tensors are derived with a simple approach. In this derivation, it is assumed that a linear relationship exists between the flux and the gradient in the transported quantity. Table 3.1 gives these linear relationships.

With the typical step sizes of the random walk of the particles along and across the magnetic field, the transport tensors can be found. In section 3.5 diamagnetic fluxes are discussed. In section 3.6 it will be explained how the transport coefficients derived in the first three sections for a simple plasma, can be generalized to more complex mixtures. Finally, in the last section, limitations of the simple approach presented in this chapter will be discussed.
A simple approach of anisotropic transport

<table>
<thead>
<tr>
<th>Property</th>
<th>Law</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion</td>
<td>Fick’s law</td>
<td>$-D \nabla n$</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Newton’s law</td>
<td>$-\eta \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right)$</td>
</tr>
<tr>
<td>Heat conduction</td>
<td>Fourier’s law</td>
<td>$-\kappa \nabla T$</td>
</tr>
</tbody>
</table>

Table 3.1: Simple laws for diffusive transport of mass, momentum and heat. Due to the magnetic field the transport coefficients in Fick’s, Newton’s and Fourier’s law will become tensors, as will be shown in this chapter.

### 3.2 Particle diffusion

Plasmas are often very complex; they consist of electrons, various types of ions, atoms and molecules. One of the simplest forms of a plasma, is a fully ionized plasma with electrons and one type of ions. Consider the motion of electrons and ions in this simple plasma. In a magnetic field, electrons and ions spiral around the field lines with the Larmor frequency $\Omega$ due to the Lorentz force. The Larmor frequency is determined by the charge $q$ of the particle, the magnetic field strength $B$ and the mass $m$ of the particle:

$$\Omega_e = \frac{q_e B}{m_e}, \quad \Omega_+ = \frac{q_+ B}{m_+}. \quad (3.1)$$

Electrons are indicated by the subscript $e$, while ions are indicated by a $+$. The spiraling motion of the electrons and ions with mean energy $\frac{3}{2} kT$ around the field lines has Larmor radius $\rho$ \(^1\), which is given by [19]:

$$\rho_e = \frac{\sqrt{2kT_e/m_e}}{\Omega_e}, \quad \rho_+ = \frac{\sqrt{2kT_+/m_+}}{\Omega_+}, \quad (3.2)$$

where $T$ is the temperature. If a particle can make more than one turn around the field line before having a collision, the particle is called magnetized. For a strongly magnetized electron in this simple plasma this means: $\Omega_e \gg \nu_{e+}$, with $\nu_{e+}$ the collision frequency between the electrons and the ions.

In a plasma without a magnetic field, diffusion is restricted by collisions. Particles can move in a certain direction until they collide with another particle. Therefore, the higher the collision frequency, the more the particle is deflected, the smaller the distance the particle can travel and thus the smaller the transport. When the electron is magnetized this situation is different. In the direction along the magnetic field the collisions still are the restricting factor in the transport. Across the magnetic field the electrons are confined within the Larmor radius around the field lines. They can only travel across

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\(^1\)This in contrast to other chapters, where $\rho$ is used for the mass density.
3.2 Particle diffusion

the magnetic field when they collide. Thus, across the field, transport is enhanced by collisions.

Figure 3.1: Diffusion of electrons. The electrons in the middle can jump to the orbit on the left or on the right when having a collision. Since there are more electrons on the left, this will result in a net electron flux to the right.

Consider figure 3.1. The spiraling electron in the middle can have a collision and then moves to the left or to the right with equal probability. Small deflections due to these collisions add up to a step $\rho_e$ in a time interval $\tau_{e^+} = 1/\nu_{e^+}$ [19]. This gives rise to a net particle flux perpendicular to the magnetic field:

$$\frac{1}{2} [n_e(x_\perp) - n_e(x_\perp + \rho_e)] \rho_e \nu_{e^+} = -\frac{\nu_{e^+}\rho_e^2}{2} \frac{\partial n_e}{\partial x_\perp},$$

(3.3)

with $n_e$ the number density of the electrons and $x_\perp$ the coordinate in the direction perpendicular to the magnetic field. Comparing this expression to Fick’s law in table 3.1, it can be seen that the diffusion perpendicular to the magnetic field is given by $D_\perp = \nu_e + \rho_e^2/2$.

In the absence of the magnetic field the stepsize of the random walk is not determined by the Larmor radius, but is given by the mean free path $\lambda_e = \nu_T \tau_{e^+}$ of the electrons, with $\nu_T$ the thermal velocity of the electrons. In the absence of a magnetic field and parallel to the magnetic field, the diffusion coefficient is therefore given by: $D = D_\parallel = \nu_e + \lambda_e^2/2$.

For the ions a similar derivation can be applied; substituting $n_+$ for $n_e$ and $\rho_+$ for $\rho_e$ gives the diffusion coefficients for the ions. Note that electron-electron and ion-ion collisions do not lead to particle transport due to conservation

2The factor $\frac{1}{2}$ in the diffusion coefficient, will appear in the viscosity and heat conduction coefficients as well. Whether this factor should be $\frac{1}{2}$ or $\frac{1}{3}$ is questionable. Here, the factor $\frac{1}{2}$ from [19] is adopted. In [1] it is pointed out that with a correct derivation this prefactor should be $\frac{1}{3}$. Since this chapter is not intended to give an exact expression, but rather an estimate of the transport coefficients, this will further be neglected.
A simple approach of anisotropic transport

of momentum. Substituting the expression found for the electron flux in equation 2.3, the following is obtained:

$$\nabla \cdot (n_e u) - \nabla \cdot \left( D_e \nabla n_e \right) = S_e,$$

(3.4)

with $D_e$ the diffusion tensor. Assuming two dimensions and a coordinate frame with directions along and across the magnetic field lines, the diffusion tensor becomes:

$$D_e = \begin{pmatrix} D_{e\parallel} & 0 \\ 0 & D_{e\perp} \end{pmatrix}.$$

(3.5)

As can be seen, perpendicular density gradients lead to perpendicular particle fluxes, while parallel density gradients lead to parallel particle fluxes. In magnetized plasmas cross terms occur as well: density gradients perpendicular to the field lines can give rise to particle fluxes around the field lines. This phenomenon is ignored here, but will be discussed in section 3.5.

### 3.3 Viscosity

For closure of the set of equations in chapter 2, an expression for the viscous stress tensor is needed. Here, a linear relationship is assumed and the coefficient of viscosity is derived. Due to the small mass of the electron, the electron viscosity can be ignored. Assume that there is a gradient in the bulk velocity $u$. The ion carries an amount $m_i u$ of momentum. The net momentum transport perpendicular to the magnetic field is therefore given by:

$$\frac{1}{2} \left[ (n_i m_i u) (x_\perp) - (n_i m_i u) (x_\perp + \rho_i) \right] \nu_i \rho_i = -\frac{\rho_i^2 n_i m_i \nu_i}{2} \frac{\partial u}{\partial x_\perp}.$$  

(3.6)

Comparing this to Newton’s law of viscosity in 3.1, it can be seen the perpendicular viscosity is given by $\frac{\rho_i^2 n_i m_i \nu_i}{2}$. Due to the fact that only ions play a role in the viscosity, the anisotropy in the viscosity will be smaller than the anisotropy in the diffusion where electrons are also taken into account. The reason is that electrons are more easily magnetized due to their small mass.

In the direction parallel to the magnetic field the stepsize of the random walk is determined by $\lambda_i = v_T \tau_i$. This gives for the viscosity coefficient:

$$\eta_\parallel = \frac{\lambda_i^2 n_i m_i \nu_i}{2}.$$  

Note that $\tau_i$ refers to momentum transfer collisions between ions.
Taking the anisotropy into account, the bulk momentum balance can now be written as:

\[ \nabla \cdot (\rho uu) = -\nabla p - \nabla \cdot \left( \eta \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot u \right) \right) + j \times B, \quad (3.7) \]

where the viscosity tensor is given by:

\[ \eta = \begin{pmatrix} \eta_\parallel & 0 \\ 0 & \eta_\perp \end{pmatrix} \quad (3.8) \]

Again the diamagnetic effect is ignored, it will be discussed in section 3.5.

### 3.4 Heat conductivity

When modeling a plasma that is not in local thermodynamic equilibrium, the electron temperature can be different from the heavy particle temperature. Therefore, both the electron and the heavy particle energy balances must be solved. As could be seen in chapter 2, the heat flux is a term that must be included in both electron and heavy particle balances. In this section the heat flux for both electrons and heavy particles in a magnetic field is derived. It is assumed that the heat flux is proportional to the temperature gradient. With the same arguments of circling motion as in 3.2, the heat conduction coefficients are found.

![Figure 3.2: Heat diffusion. The number of electrons moving from left to right is the same as the number of electrons moving from right to left. Due to the temperature gradient, there will be a heat flux. Since the Larmor radius increases with increasing temperature, the circles towards the left increase in size.](image)

Assume that there is a temperature gradient, but no density gradient, see figure 3.2. Again the electron in the middle can make a jump to the left or the right due to collisions. The electron carries an amount \( \frac{3}{2} k_B T_e \) of energy.
The net energy transport or heat flux perpendicular to the magnetic field $q_{e\perp}$ is therefore given by:

$$q_{e\perp} = \frac{13}{2} \left[ (n_e k_B T_e) (x_\perp) - (n_e k_B T_e) (x_\perp + \rho_e) \right] \nu_e \rho_e = -\frac{3 \rho_e^2 \nu_e n_e k_B \partial T_e}{4 \partial x_\perp}. \quad (3.9)$$

The heat conductivity can thus be written as: $\kappa_\perp = \frac{3 \nu_e^2 n_e k_B}{4}$. Parallel to the magnetic field, the mean free path is $\lambda_e$. Therefore, the heat conductivity along the magnetic field becomes $\kappa_\parallel = \frac{3 \lambda_e^2 \nu_e n_e k_B}{4}$. Attention has to be paid to the fact that in heat conduction, collisions between two identical particles do lead to a heat flux. Therefore, $\nu_e$ contains the contributions of electron-electron collisions. This is in contrast with diffusion, where collisions between identical particles do not contribute to the diffusion coefficient because of conservation of momentum. For the ions, the heat conductivity can be derived in a similar way as for the electrons.

With the calculated heat conduction tensors, the electron energy balance from chapter 2 becomes:

$$\nabla \cdot (C_e T_e u_e) + p_e \nabla \cdot u_e - \nabla \cdot (\kappa \nabla T_e) = Q_{\text{ohm}} + Q_e, \quad (3.10)$$

where $\kappa$ is the heat conduction tensor. Assuming two dimensions and a coordinate frame with directions along and across the magnetic field lines, the heat conduction tensor becomes:

$$\kappa = \begin{pmatrix} \kappa_\parallel & 0 \\ 0 & \kappa_\perp \end{pmatrix} \quad (3.11)$$

Note that diamagnetic effects are again ignored. They are discussed in the next section.

### 3.5 Diamagnetic fluxes

In a plasma without magnetic field, a gradient drives a flux opposite to that gradient. For example, a density gradient that points radially inward will drive a particle flux that points radially outward. In a magnetized plasma the situation is different. Still, a gradient drives a flux opposite to that gradient. But in the directions across and around the magnetic field lines, a gradient also drives a flux perpendicular to that gradient. For example, a radial density gradient, can cause an azimuthal particle flux when the magnetic field points in the axial direction. These fluxes are called diamagnetic fluxes and
3.6 Partially magnetized species

are caused by the circling motion of the charged particles. The mechanism that causes diamagnetic fluxes is schematically depicted in figure 3.3. The more electrons, the thicker the line in this figure. Where two circles meet, more electrons are moving in upward direction, since there are more electrons on the left circle.

![Diamagnetic fluxes](image)

Figure 3.3: Diamagnetic fluxes. The electron density gradient causes an electron flux perpendicular to the gradient.

In the previous sections it was assumed that the plasma was two dimensional and diamagnetic effects were ignored. To take the diamagnetic effect into account 3 dimensions must be regarded. In a coordinate system with directions along, across and around the magnetic field lines, the diamagnetic terms appear as off-diagonal elements in the derived transport tensors:

\[
\kappa = \begin{pmatrix}
\kappa_\parallel & 0 & 0 \\
0 & \kappa_\perp & \kappa_{\text{dia}} \\
0 & \kappa_{\text{dia}} & \kappa_\wedge
\end{pmatrix}
\]  (3.12)

As can be seen, the parallel transport is not influenced by the diamagnetic effect. In a cylindrical plasma where the magnetic field points in axial direction, like in Pilot and Magnum PSI, a radial ion density gradient will drive a current in the azimuthal direction. This current must be taken into account in the \( \vec{j} \times \vec{B} \) term in the bulk momentum balance, since it influences the radial velocity. This azimuthal current must also be taken care of when looking at ambipolar diffusion in a magnetic field. This will be discussed in section 4.3.

### 3.6 Partially magnetized species

The transport coefficients in section 3.2, 3.3 and 3.4 were derived for a plasma consisting of electrons and ions. It was shown that for diffusion, only electron-ion interactions are important; that for heat conduction, electron-electron
and ion-ion interactions have to be taken into account, whereas for the calculation of the viscosity ion-ion and ion-electron interactions have to be dealt with. In general, there are more species involved; apart from electrons and ions plasmas may also contain (excited) atoms and molecules. Therefore, more interactions have to be taken into account. In this section, a sketch is given of the generalization of the transport tensors to more complex mixtures and to the case where the plasma is not fully magnetized. The heavy particle thermal conductivity is taken as an example.

In the preceding sections it was shown that parallel transport was decreased by collisions, while perpendicular transport was enhanced by collisions when the plasma was fully magnetized. But often the plasma is not fully magnetized. Especially ions require a large magnetic field and a low pressure before becoming magnetized. It can also occur that the ions and electrons are magnetized, but that there are also neutrals that contribute to the transport perpendicular to the field. How can these effects be taken into account in a more general plasma?

Regard the contribution of one species (e.g. electron, ion) perpendicular to the field: $\kappa_{i\perp}$. There is a simple way to avoid the problems with non fully magnetized species or neutrals by defining this perpendicular contribution as:

$$\kappa_{i\perp} = \frac{1}{1 + (\omega \tau_i)^2 \kappa_{i\parallel}}. \quad (3.13)$$

When there is no magnetic field, this expression yields the parallel conductivity. When the species is fully magnetized ($\omega \tau_i \gg 1$), this expression reduces to the expression given in section 3.4. For the heavy particle heat conductivity, these individual contributions can now be summed over the heavy particles to obtain the total heavy particle heat conductivity:

$$\kappa_{\text{heavy}\perp} = \sum_i \kappa_{i\perp}. \quad (3.14)$$

### 3.7 Limitations of a simple approach

In chapter 2, the equations solved in Plasimo were presented. For closure of this set of equations, expressions for species, momentum and heat flux are needed. In this chapter expressions for these fluxes in a magnetic field were found. It was assumed that the linear relationships of table 3.1 were valid. These are, however, only approximations of the fluxes. There is a fundamental difference between the species flux on the one hand and the
momentum and heat flux on the other hand. The momentum and heat flux can only be approximated, while the species flux can be determined with the species momentum balance. In fact, Fick’s law is a simplification of the full species momentum balance and is valid when there is a dominant background species in the absence of temperature gradients and electric fields. These are restrictions that are generally not met in a plasma, and certainly not in the plasma of interest. For that reason, in the next chapter a more complete diffusion description is given in the presence of a magnetic field.
A simple approach of anisotropic transport
Chapter 4

Self consistent diffusion in a magnetic field

4.1 Introduction

In chapter 3, a simplified theory was presented for the diffusion in a magnetized plasma. This theory was based on the assumption that the cumulative effect of all collisions in a time interval $\tau$ results in an average displacement of a charged particle of one Larmor radius perpendicular to the magnetic field and one mean free path parallel to the magnetic field. This simplified description of diffusion is only valid in the case of diffusion of one type of particle through a dominant background gas with constant density and temperature. To describe more complex plasmas, the specific momentum balance for all species $i$ must be considered [18, 33].

In section 4.2, starting from the full momentum balances, diffusion equations are derived that are suitable for implementation in Plasimo. The derived equations are compared to diffusion equations in literature. In section 4.3, ambipolar diffusion in a magnetic field is discussed and an expression for the ambipolar electric field in a magnetic field is derived. Section 4.4 shows that in limiting cases the diffusion equations of this chapter reduce to the simplified approach of chapter 3.

4.2 Derivation of the diffusion equations

For modeling of multi-component plasmas, a description of the different species in the plasma is often wanted. This description can be given in terms of the species distribution functions. These functions give the position
of the different species in phase space. In this context, a species can be an electron, atom, ion or molecule with a certain internal structure [5]. Hence, atoms, ions and molecules with different excitation states are considered to be different species.

The species distribution function \( f_i(r, v, t) \) is defined such that \( f_i(r, v, t) drd\mathbf{v} \) is the number of particles of species type \( i \) within a volume element \( dr \) around \( r \) within velocity space element \( d\mathbf{v} \) around \( \mathbf{v} \) at time \( t \). The evolution of the distribution function in time can be described by the Boltzmann transport equation [4, 20]:

\[
\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_r f_i + \frac{\mathbf{F}_i}{m_i} \cdot \nabla_v f_i = \left( \frac{\partial f_i}{\partial t} \right)_e, \tag{4.1}
\]

where the first term on the lhs represents the temporal evolution, the second term the change because of spatial gradients and the third term describes the change in the distribution function due to forces \( \mathbf{F}_i \) acting on the species of mass \( m_i \). The nabla operator in position space is denoted by \( \nabla_r \), whereas \( \nabla_v \) gives the nabla operator in velocity space. The rhs gives the change in the distribution function due to elementary processes like excitation and de-excitation.

Mass, momentum and energy conservation equations for the species in a plasma can be obtained from the Boltzmann transport equation. This is done by multiplying the Boltzmann transport equation with functions of the velocity and integrating the expression over velocity space. These functions are \( m_i \) for the mass conservation equation (the zeroth moment), \( m_i \mathbf{v} \) for the momentum conservation equation (the first moment) and \( \frac{1}{2} m_i \mathbf{v}^2 \) for the energy conservation equation (the second moment). For the derivation of the self consistent diffusion equations, the momentum balance is of special interest.

**The momentum balance for each species** To obtain the momentum balance of species \( i \), the first moment of the Boltzmann transport equation must be taken. The derivation will not be carried out here, instead the result of [5, 20, 41] is used. In steady state, the momentum balance reads:

\[
\nabla \cdot (\rho_i \mathbf{u}_i \mathbf{u}_i) = -\nabla \cdot \mathbf{F}_i^m + \mathbf{R}_i^F + \mathbf{F}_i, \tag{4.2}
\]

with \( \rho_i = n_i m_i \) the mass density of species \( i \), \( \mathbf{u}_i \) the average velocity of species \( i \). Therefore, the first term on the left hand side gives the advection
of momentum\(^1\). The pressure tensor of species \(i\) is defined as \(\overline{P}_i^* = \rho_i \langle \mathbf{c}_i \mathbf{c}_i \rangle\), with \(\mathbf{c}_i\) the peculiar velocity with respect to the mean velocity of species \(i\), while the integration over velocity space is denoted by \(\langle \rangle\). The pressure tensor contains both the scalar pressure and viscous forces. The term \(R_i^F\) is the friction force and gives the momentum exchange between species \(i\) and all the other species due to collisions. The term \(F_i\) represents the volume forces, for example, the electric field, magnetic field or gravitational field.

**Transformation to the bulk system** The pressure tensor as used in equation 4.2 is defined in the system of species \(i\) and gives the rate at which momentum is transferred across a surface moving with the mean velocity \(\mathbf{u}_i\) of the species. In contrast, the bulk pressure tensor \(\overline{P}_i\) gives the rate at which momentum is transferred across a surface moving with the mass averaged velocity \(\mathbf{u}\). This has the consequence that summation of \(\overline{P}_i^*\) over all species \(i\) does, in general, not give the total pressure tensor \(\overline{P}\). The specific pressure tensor can be transformed to the bulk system via \([4, 20]\):

\[
\overline{P}_i^* = \overline{P}_i - \rho_i \mathbf{v}_i \mathbf{v}_i,
\]

(4.3)

where \(\mathbf{v}_i = \mathbf{u}_i - \mathbf{u}\) is the averaged diffusion velocity of species \(i\) and \(\overline{P}_i\) the pressure tensor of species \(i\) with respect to the bulk frame. If this transformed pressure tensor is summed over all the species it yields the total pressure:

\[
\sum_i \overline{P}_i = \overline{P}.
\]

(4.4)

Decomposing the average velocity in a bulk and diffusion velocity \(\mathbf{u}_i = \mathbf{u} + \mathbf{v}_i\) and substituting the new pressure tensor in the specific momentum balance leads to:

\[
\nabla \cdot (\rho_i \mathbf{u} \mathbf{u}) + \nabla \cdot (\rho_i \mathbf{u} \mathbf{v}_i) + \nabla \cdot (\rho_i \mathbf{v}_i \mathbf{u}) =
- \nabla \cdot \overline{P}_i + R_i^F + F_i.
\]

(4.5)

**Substitution of the bulk momentum balance** It can be shown \([5, 20]\) that summation of the *transformed* species balances 4.5 over all species \(i\) leads to the bulk momentum balance:

\[
\rho \mathbf{u} \cdot (\nabla \mathbf{u}) = - \nabla \cdot \overline{P} + \mathbf{F}.
\]

(4.6)

\(^1\)Note that in literature this term is sometimes replaced by \(\rho_i \mathbf{u}_i \cdot \nabla \mathbf{u}_i\). This is possible, provided that the change in momentum due to the creation of species in chemical reactions can be neglected.
This bulk momentum balance can be used to substitute the term $\rho_i uu$ in the specific momentum balance. To this end, the first term of equation 4.5 is manipulated by rewriting the dyadic product as:

$$\nabla \cdot (\rho_i uu) = [\nabla \cdot (\rho_i u)] u + \rho_i u \cdot (\nabla u).$$

(4.7)

Returning to equation 4.5 and using the obtained expression for $\nabla \cdot (\rho_i uu)$, the species momentum now can be written as:

$$\begin{align*}
[\nabla \cdot (\rho_i u)] u &+ \rho_i u \cdot (\nabla u) + \nabla \cdot (\rho_i uv_i) \\
+ \nabla \cdot (\rho_i v_i u) & = -\nabla \cdot \vec{P} + \text{R}_1^F + \text{F}_1.
\end{align*}$$

(4.8)

Using the bulk momentum balance 4.6, the second term can be written as:

$$y_i \rho u \cdot (\nabla u) = -y_i \nabla \cdot \vec{P} + y_i \text{F}.$$  

(4.9)

By substitution of this bulk momentum balance and some manipulation of the inertial terms, equation 4.8 can be transformed to:

$$
\begin{align*}
&[\nabla \cdot (\rho_i u)] u + [\nabla \cdot (\rho_i uv_i)] + \rho_i v_i \cdot \nabla u \\
= & -\nabla \cdot \vec{P} + \text{R}_1^F + \text{F}_1 + y_i \nabla \cdot \vec{P} - y_i \text{F}.
\end{align*}
$$

(4.10)

**Comparison to literature** If equation 4.10 is compared to diffusion equations in literature, the following points attract attention:

- **Term 4** Viscosity, which is the friction between like particles, is often neglected in diffusion equations [9, 26, 33, 34, 40], resulting in $-\nabla \cdot \vec{P}_i + y_i \nabla \cdot \vec{P}$ being replaced by $-\nabla p_i + y_i \nabla p$.

- **Term 7 and 8** are not always taken into account [9, 26, 37]. When there is no bulk flow and the motion of the species is purely diffusional this is permitted. However, when the bulk flow is not zero, omitting this term can give problems. Note that term 7 and 8 can be found in the equations of [33], but that they are derived by assuming that the species velocity $u_i$ is nearly equal to the bulk velocity $u$. In many plasmas, this is not a valid assumption.
4.2 Derivation of the diffusion equations

- **Term 1, 2 and 3**, the inertial terms, are often neglected. Since term 1 can be interpreted as the momentum created in chemical reaction advected by the bulk flow, omittance of term 1 can be justified when elastic collisions are dominant over inelastic collisions as is shown in [23]. Cross terms of diffusion and bulk velocity (term 2 and 3) can be neglected in the large friction limit [33, 34, 35], when the diffusion velocity is much smaller than the bulk velocity.

In the expansion of Magnum PSI, both bulk plasma flow (the expansion into a low pressure chamber) and diffusion (invasion of neutrals into the plasma beam) are important. Furthermore, both in the source and in the expansion, the assumption of large friction seems not to be justified. In the arc the bulk flow is mainly in the axial direction, while the diffusion takes place in the radial direction. In the expansion chamber the pressure is very low. It thus seems, that the assumptions that are usually made in diffusion equations do not hold for Magnum PSI. A multi fluid approach like in [28], where the complete specific species mass and momentum balances are solved by the SIMPLE algorithm\(^2\) seems to be better suited. However, applying the SIMPLE algorithm in a situation where velocity components are coupled via the Lorentz force might not be possible. Furthermore, in the current setup of Plasimo, the bulk flow is solved with the SIMPLE algorithm and the species velocities are described by simplified diffusion equations. To make use of this existing framework of diffusion equations, terms 1, 2, 3 and 8 are neglected, and only the pressure is taken into account in term 4 and 7.

**Simplified diffusion equations**  With the above simplifications, equation 4.10 reduces to:

\[
- \nabla p_i + F_i + R_i^F + y_i \nabla p = 0. \tag{4.11}
\]

Neglecting the gravitational force, the force \(F_i\) can be written as:

\[
F_i = n_i q_i E + n_i q_i u_i \times B, \tag{4.12}
\]

where \(n_i\) is the number density of species \(i\), \(q_i\) its charge, \(E\) the electric field and \(B\) the magnetic field. Substitution of equation 4.12 into equation 4.11 gives:

\[
- \nabla p_i + n_i q_i E + n_i q_i u_i \times B + R_i^F + y_i \nabla p = 0. \tag{4.13}
\]

\(^2\)The SIMPLE algorithm is an algorithm to solve the coupled set of continuity and momentum equations to obtain the flow field. The SIMPLE algorithm will be discussed in chapter 6.
The friction force $R_i^F$ is defined as:

$$R_i^F = \sum_j f_{ij} (u_j - u_i), \quad (4.14)$$

with $f_{ij}$ the volumetric friction force per unit of velocity difference:

$$f_{ij} = n_i n_j m_{ij} \Omega_{ij}, \quad (4.15)$$

where $\Omega_{ij}$ is the rate coefficient for momentum transfer from species $i$ to $j$ and $m_{ij}$ the reduced mass of the $i, j$-system. The force balance now becomes:

$$-\nabla p_i + n_i q_i E + n_i q_i u_i \times B + \sum_j f_{ij} (u_j - u_i) + y_i \nabla p = 0 \quad (4.16)$$

When $f_i^{eff}$ is defined as $f_i^{eff} = \sum_j f_{ij}$ this can be written as:

$$f_i^{eff} u_i = \sum_j f_{ij} u_j - \nabla p_i + n_i q_i E + n_i q_i u_i \times B + y_i \nabla p. \quad (4.17)$$

The momentum balances give a set of $N$ equations for the diffusive velocities, with $N$ the number of species. Only $N - 1$ of these equations are independent, since summation over the species velocities should give the bulk flow velocity. Furthermore, it must be realized that the electric field that occurs in the force balance is an unknown in the diffusion problem. An expression for the electric field must be found. In a plasma the electric field consists of contributions of both externally applied fields and the ambipolar field. Calculation of the ambipolar field in a plasma in a magnetic field is not so straightforward and will be discussed in the next section.

### 4.3 Ambipolar diffusion in a magnetic field

For calculation of the ambipolar field in the presence of a magnetic field, distinction must be made between the directions along, across and around the magnetic field lines. Therefore, the momentum balances are split up in components along (||), across (∥) and around (∧) the magnetic field:

$$f_i^{eff} u_{i\perp} = \sum_j f_{ij} u_{j\perp} - \frac{\partial p_i}{\partial \perp} + n_i q_i u_{i\perp} B + n_i q_i E_{\perp} + y_i \frac{\partial p}{\partial \perp}, \quad (4.18)$$

$$f_i^{eff} u_{i\wedge} = \sum_j f_{ij} u_{j\wedge} - \frac{\partial p_i}{\partial \wedge} - n_i q_i u_{i\perp} B + n_i q_i E_{\wedge} + y_i \frac{\partial p}{\partial \wedge}. \quad (4.19)$$
4.3 Ambipolar diffusion in a magnetic field

\[
f_i^{\text{eff}} u_{i\parallel} = \sum_j f_{ij} u_{j\parallel} - \frac{\partial p_i}{\partial \parallel} + n_i q_i E\parallel + y_i \frac{\partial p}{\partial \parallel}. \tag{4.20}
\]

Normally, without a magnetic field, the ambipolar field \( E_a \) is calculated as the electric field that is necessary to prevent charge separation\(^3\). This calculation will be applied along and across the magnetic field. Around the field lines, it is impossible for the electrons and ions to diffuse together. This can be explained with figure 4.1. In the cylindrically symmetric plasma there is a radial gradient of charged particles. The magnetic field points out of the plane. Because of the opposite charge of the electrons and ions, the circling motion of the electrons is in the opposite direction of the motion of the ions. This means that their contribution to the current has the same sign, which is the mechanism behind the diamagnetic current\(^4\).

![Diamagnetic current as a result of a radial density gradient. As long as there is a magnetic field, this diamagnetic current cannot be zero.](image)

For the direction around the field lines, the external electric field \( E_J \), the gradients of temperature and pressure and the interaction term with other

---

\(^3\)When there is an externally applied electric field, there is separation because there is a current. To calculate the ambipolar field in this situation, the external field and the current must be set to zero.

\(^4\)This diamagnetic current will also induce a magnetic field. This effect will be neglected here.
species are set to zero, which gives:

\[ f_{i}^{\text{eff}} u_{i\parallel} = -n_{i} q_{i} u_{i\perp} B. \]  
(4.21)

Note that this is a simplification, since the friction between species is neglected. By substitution of the equation, the balance in the \( \perp \) direction becomes:

\[ \left( f_{i}^{\text{eff}} + \frac{n_{i}^{2} q_{i}^{2} B^{2}}{f_{i}^{\text{eff}}} \right) u_{i\perp} = \sum_{j} f_{ij} u_{j\perp} - \frac{\partial p_{i}}{\partial \perp} + n_{i} q_{i} E_{\perp} + y_{i} \frac{\partial p}{\partial \perp} \]  
(4.22)

The ambipolar field in the direction across the magnetic field will now be determined by the restriction that the current in that direction is zero:

\[ J_{\perp} = \sum_{i} n_{i} q_{i} u_{i\perp} = \sum_{i} \frac{n_{i} q_{i}}{f_{i}^{\text{eff}} + \frac{n_{i}^{2} q_{i}^{2} B^{2}}{f_{i}^{\text{eff}}}} \left( \sum_{j} f_{ij} u_{j\perp} - \frac{\partial p_{i}}{\partial \perp} + n_{i} q_{i} E_{\perp} + y_{i} \frac{\partial p}{\partial \perp} \right) = 0 \]  
(4.23)

This implies that the ambipolar field must be given by:

\[ E_{a\perp} = \frac{1}{\sigma_{\perp}} \sum_{i} \mu_{i\perp} \left( - \sum_{j} f_{ij} u_{j\perp} + \frac{\partial p_{i}}{\partial \perp} - y_{i} \frac{\partial p}{\partial \perp} \right), \]  
(4.24)

where the mobility and the conductivity perpendicular to the magnetic field are introduced:

\[ \mu_{i\perp} = \frac{n_{i} q_{i}}{f_{i}^{\text{eff}} + \frac{n_{i}^{2} q_{i}^{2} B^{2}}{f_{i}^{\text{eff}}}}, \quad \sigma_{\perp} = \sum_{i} n_{i} q_{i} \mu_{i\perp}. \]  
(4.25)

Note that for negatively charged species, the mobility is negative, whereas the conductivity is always positive.

**The direction of the ambipolar field** Equation 4.24 shows an interesting phenomenon of ambipolar diffusion in a magnetic field: depending on the strength of the magnetic field, the ambipolar field can be both positive and negative. This can be demonstrated as follows: assume that the friction with other species can be neglected and that the total pressure is uniform\(^5\) in

---

\(^5\)Including the friction and pressure term in the ambipolar field expression, makes the phenomenon less apparent. It does however not change the conclusion that the sign of the ambipolar field can be reversed in a magnetic field.
equation 4.24. Furthermore, assume that the partial pressure of the electrons and the ions is larger in the center of the discharge than at the wall. Now two cases can be considered:

1. With small magnetic fields, the absolute value of the mobility of the electrons is larger than the mobility of the ions, because \( f_{eff} \) is small, due to the small mass of the electrons. The radial gradients of the partial pressures of the electrons and ions are equal in size and negative. From equation 4.24, it can be seen that in this situation, the ambipolar field points in the positive radial direction.

2. As the magnetic field strength increases, the absolute value of the electron mobility decreases as can be seen in (4.25). When the magnetic field is strong enough, the electron mobility can even become smaller than the ion mobility. As a result, the ambipolar field changes sign and points in the negative radial direction.

Parallel to the magnetic field, the mobility and conductivity are given by the following expressions:

\[
\mu_{||} = \frac{n_i q_i}{f_i^{eff}}, \quad \sigma_{||} = \sum_i n_i q_i \mu_{||}, \tag{4.26}
\]

and the ambipolar field is given by:

\[
E_{a||} = \frac{1}{\sigma_{||}} \sum_i \mu_{||} \left( - \sum_j f_{ij} u_{j||} + \frac{\partial p_i}{\partial ||} - y_i \frac{\partial p}{\partial ||} \right). \tag{4.27}
\]

As can be seen, the expressions for the ambipolar field parallel and perpendicular to the magnetic field have a similar structure. Substitution of the ambipolar fields into the momentum balances parallel and perpendicular to the magnetic field gives:

\[
\left( f_i^{eff} + \frac{n_i q_i^2 B^2}{f_i^{eff}} \right) u_{i\perp} - \sum_j f_{ij} u_{j\perp} + \frac{n_i q_i}{\sigma_{\perp}} \sum_j \mu_{j\perp} \sum_k f_{jk} u_{k\perp} = -\frac{\partial p_i}{\partial \perp} \\
+ \frac{n_i q_i}{\sigma_{\perp}} \sum_j \mu_{j\perp} \frac{\partial p_j}{\partial \perp} + n_i q_i E_{J\perp} + y_i \frac{\partial p}{\partial \perp} - \frac{n_i q_i}{\sigma_{\perp}} \sum_j \mu_{j\perp} y_j \frac{\partial p}{\partial \perp} \tag{4.28}
\]

and
These momentum balances for each species form a coupled set of equations for the velocities. As will be shown in chapter 5, this can be written as a matrix vector equation, which is suitable for implementation in Plasimo. In the following section it is shown that under certain assumptions the self consistent diffusion equations reduce to the simple approach as presented in chapter 3.

4.4 Reduction to the simple approach

In 3.2 and section 4.2 two different approaches for calculation of diffusion in a magnetized plasma were presented: a simple approach based on the stepsize in collisions and the more sophisticated approach of self consistent diffusion. In this section it will be shown that the self consistent diffusion equations reduce to the simple approach when certain assumptions are made. These assumptions are:

- There is no temperature gradient, partial pressure gradients can thus be written as number density gradients.
- There is no bulk flow and hence, there is no bulk pressure gradient; this implies that terms with \( y_i \) in (4.28) and (4.29) can be eliminated.
- There is no externally applied electric field, so \( E_J \) is zero in (4.28) and (4.29).
- The species diffuse through a fixed, homogeneous background gas of neutral particles. The velocity of this background gas can thus be neglected.

The ambipolar diffusion of electrons and ions is considered. With the above assumptions, equation 4.28 and 4.29 for the electrons reduce to:

\[
f_{\text{eff}}^{\text{e}} u_e = - \frac{\partial p_e}{\partial \parallel} + \frac{n_e q_e}{\sigma_{\parallel}} \sum_j \mu_{j\parallel} \frac{\partial p_j}{\partial \parallel} \tag{4.30}\]

\[
f_{\text{eff}}^{\text{i}} u_i = - \frac{\partial p_i}{\partial \parallel} + \frac{n_i q_i}{\sigma_{\parallel}} \sum_j \mu_{j\parallel} \frac{\partial p_j}{\partial \parallel} + n_i q_i \sigma_{\parallel} \sum_j \mu_{j\\parallel} y_j \frac{\partial p_j}{\partial \parallel}.	ag{4.29}
\]
4.4 Reduction to the simple approach

\[
\left( f_{\text{eff}} + \frac{n_e^2 e^2 B^2}{f_{\text{eff}}^2} \right) u_{e\perp} = -\frac{\partial p_e}{\partial \perp} + n_e q_e \sum_j \mu_{j\perp} \frac{\partial p_j}{\partial \perp} \quad (4.31)
\]

Multiplying both equations with the electron mobility \((\mu_{e\parallel}, \mu_{e\perp})\) and writing down the ambipolar term gives:

\[
n_e q_e u_{e\parallel} = \mu_{e\parallel} \left[ -\frac{\partial p_e}{\partial \parallel} + \frac{n_e q_e}{\sigma_{\parallel}} \left( \mu_{e\parallel} \frac{\partial p_e}{\partial \parallel} + \mu_{e\perp} \frac{\partial p_e}{\partial \parallel} \right) \right] \quad (4.32)
\]

and

\[
n_e q_e u_{e\perp} = \mu_{e\perp} \left[ -\frac{\partial p_e}{\partial \perp} + \frac{n_e q_e}{\sigma_{\perp}} \left( \mu_{e\perp} \frac{\partial p_e}{\partial \perp} + \mu_{e\parallel} \frac{\partial p_e}{\partial \parallel} \right) \right]. \quad (4.33)
\]

Putting together both terms with the electron pressure and making use of the definitions of the conductivity 4.25 and 4.26 leads to:

\[
n_e q_e u_{e\parallel} = -\mu_{e\parallel} \left[ \frac{n_e q_e + \mu_{e\parallel}}{\sigma_{\parallel}} \left( \frac{\partial p_e}{\partial \parallel} + \frac{\partial p_e}{\partial \perp} \right) \right] \quad (4.34)
\]

and

\[
n_e q_e u_{e\perp} = -\mu_{e\perp} \left[ \frac{n_e q_e + \mu_{e\perp}}{\sigma_{\perp}} \left( \frac{\partial p_e}{\partial \parallel} + \frac{\partial p_e}{\partial \perp} \right) \right]. \quad (4.35)
\]

For the direction along the magnetic field lines it is assumed that the electrons are much more mobile than the ions, leading to:

\[
n_e q_e u_{e\parallel} = \mu_{e\parallel} \left( \frac{\partial p_e}{\partial \parallel} + \frac{\partial p_e}{\partial \perp} \right) \quad (4.36)
\]

In the direction perpendicular to the magnetic field it is assumed that the plasma is strongly magnetized, and thus that the mobility of the ions is much larger than the mobility of the electrons:

\[
n_e q_e u_{e\perp} = -\mu_{e\perp} \left( \frac{\partial p_e}{\partial \parallel} + \frac{\partial p_e}{\partial \perp} \right) \quad (4.37)
\]

The Einstein relation between mobility and diffusion coefficient is given by:

\[
\mu_{e\parallel} = \frac{q_e D_{e\parallel}}{kT_e}, \quad \mu_{e\perp} = \frac{q_e D_{e\perp}}{kT_e}. \quad (4.38)
\]

If this Einstein relation is used, together with the assumption of quasi-neutrality \((n_e = n_+)\), the ambipolar flux of electrons can be written as follows:
The flux of electrons parallel to the magnetic field reduces to the classical expression of ambipolar diffusion [18]. Both the electrons and the ions diffuse with the mobility of the ions and the temperature of the electrons. As can be seen, in the case of diffusion perpendicular to the magnetic field, the equation looks quite similar. However, the situation is reversed: the electrons and ions diffuse with the mobility of the electrons and the temperature of the ions. Writing out the expressions for the diffusion coefficients, the following result is found:

\[
D_+ = \frac{kT_+ \mu_+}{q_+} = \frac{kT_+ n_+}{f^{\text{eff}}_+} = \frac{kT_+}{m_0 \nu_{+0}} \propto \lambda_+^2 \nu_{+0}
\]

and

\[
D_e = \frac{kT_e \mu_e}{q_e} = \frac{kT_e n_e f^{\text{eff}}_e}{q_e n_e^2 q_e^2 B^2} = \frac{kT_e m_e \nu_{e0}}{q_e^2 B^2} \propto \rho_e^2 \nu_{e0},
\]

where \(\nu_{+0}\) is the collision frequency for the ions with the background gas and \(\nu_{e0}\) is the collision frequency for the electrons with the background gas. Note the similarity with the result derived in section 3.2. The diffusion coefficient scales with the mean free path parallel to the magnetic field and with the Larmor radius perpendicular to the magnetic field.
Chapter 5

Implementation and validation of anisotropic diffusion

5.1 Implementation in Plasimo

In chapter 4, self consistent diffusion equations (equations 4.28 and 4.29) in the presence of a magnetic field were derived. These self consistent diffusion equations yield a coupled set of equations for the total velocities of all the species in the plasma. For each velocity component, the diffusion equations can be written in matrix vector representation as follows:

\[ Av = b, \] (5.1)

where matrix \( A \) contains the frictional terms with \( f_{\text{eff}}^i \) and \( f_{ij} \), vector \( v \) contains one component of the velocities \( u_i \) for all species and vector \( b \), contains the driving mechanisms for diffusion. In the derivation of the diffusion equation perpendicular to the magnetic field, the force balance in the direction around the field lines was substituted in the force balance perpendicular to the magnetic field. This implies that the matrix vector equations have to be solved only for the directions perpendicular and parallel to the magnetic field: the information of the equation around the field lines is implicitly present in the equation perpendicular to the magnetic field.

The species velocities should be consistent with the bulk velocity. Therefore, the coupled set of diffusion equations is solved under the constraint:

\[ \sum_i n_i m_i u_i = \rho u. \] (5.2)

This constraint is taken into account by replacing the diffusion equation for the "zeroth" particle by equation 5.2. This leads to the following expressions:
Implementation and validation of anisotropic diffusion

\[
\begin{align*}
A_\perp \begin{pmatrix}
u_0 \perp \\
u_1 \perp \\
u_2 \perp \\vdots \\
u_N \perp 
\end{pmatrix} = b_\perp & \quad A_\parallel \begin{pmatrix}
u_0 \parallel \\
u_1 \parallel \\
u_2 \parallel \\vdots \\
u_N \parallel 
\end{pmatrix} = b_\parallel \\
\begin{pmatrix}ho u_1 \\
b_1 \parallel \\
b_2 \parallel \\
\vdots \\
b_N \parallel 
\end{pmatrix} = b_\parallel & \quad \begin{pmatrix}ho u_1 \perp \\
b_1 \perp \\
b_2 \perp \\
\vdots \\
b_N \perp 
\end{pmatrix} = b_\perp
\end{align*}
\]

\[
b_i \parallel = n_i q_i E_j \parallel - \frac{\partial p_i}{\partial \parallel} + y_i \frac{\partial p}{\partial \parallel} + \frac{n_i q_i}{\sigma_\parallel} \sum_j \mu_j \parallel \left( \frac{\partial p_j}{\partial \parallel} \right) - \frac{n_i q_i}{\sigma_\parallel} \sum_j \mu_j \parallel y_j \frac{\partial p}{\partial \parallel}
\]

\[
b_i \perp = n_i q_i E_j \perp - \frac{\partial p_i}{\partial \perp} + y_i \frac{\partial p}{\partial \perp} + \frac{n_i q_i}{\sigma_\perp} \sum_j \mu_j \perp \left( \frac{\partial p_j}{\partial \perp} \right) - \frac{n_i q_i}{\sigma_\perp} \sum_j \mu_j \perp y_j \frac{\partial p}{\partial \perp}
\]
5.1 Implementation in Plasimo

\[ A\parallel = \begin{pmatrix} n_0m_0 & n_1m_1 & n_2m_2 & \cdots & n_Nm_N \\ a_{10\parallel} & a_{11\parallel} & a_{12\parallel} & \cdots & a_{1N\parallel} \\ a_{20\parallel} & a_{21\parallel} & a_{22\parallel} & \cdots & a_{2N\parallel} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{N0\parallel} & a_{N1\parallel} & a_{N2\parallel} & \cdots & a_{NN\parallel} \end{pmatrix} \]

\[ A\perp = \begin{pmatrix} n_0m_0 & n_1m_1 & n_2m_2 & \cdots & n_Nm_N \\ a_{10\perp} & a_{11\perp} & a_{12\perp} & \cdots & a_{1N\perp} \\ a_{20\perp} & a_{21\perp} & a_{22\perp} & \cdots & a_{2N\perp} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{N0\perp} & a_{N1\perp} & a_{N2\perp} & \cdots & a_{NN\perp} \end{pmatrix} \]

\[ a_{ij\parallel} = \begin{cases} -f_{ij} + \frac{n_iq_i}{\sigma_{\parallel}} \sum_k f_{ki}\mu_k & \text{if } i \neq j \\ f_{i\text{eff}} + \frac{n_iq_i}{\sigma_{\parallel}} \sum_k f_{ki}\mu_k & \text{if } i = j \end{cases} \]

\[ a_{ij\perp} = \begin{cases} -f_{ij} + \frac{n_iq_i}{\sigma_{\perp}} \sum_k f_{ki}\mu_k & \text{if } i \neq j \\ f_{i\text{eff}} + \frac{n_i^2q_i^2B^2}{f_{i\text{eff}}} + \frac{n_iq_i}{\sigma_{\perp}} \sum_k f_{ki}\mu_k & \text{if } i = j \end{cases} \]
Implementation and validation of anisotropic diffusion

The matrix-vector equations are solved with either the Gauss-Jordan or Singular Value Decomposition method as explained in [18]. In contrast to [18], the solution of the system does not yield the diffusion velocity, but the total velocity $u_i$ of each species. This is transformed to a diffusion velocity via:

$$v_i = u_i - u,$$

which is again transformed to:

$$v^*_i = v_i + \frac{D_i}{n_i} \nabla n_i.$$

The last transformation is carried out for numerical stability [18], since it is difficult to solve the $\phi$ equation without diffusion terms. The species densities now follow from:

$$\nabla \cdot \left( n_i (u + v^*_i) \right) - \nabla \cdot (D_i \nabla n_i) = S_i.$$

It appears that this formulation of the species balance gives problems when a temperature gradient is present. This is discussed in chapter 8.

5.2 Validation

As was derived in section 4.4, diffusion of charged species through a dominant background gas without temperature gradients or an externally applied electric field can be described with a single ambipolar diffusion coefficient. In this section, the equilibrium between production and diffusion of electrons is studied. This is done for a situation in which an analytical expression for the electron density can be derived. In this way, the anisotropic diffusion implementation can be validated by comparing the model results with the analytical expression.

**Analytical solution of the test case** For derivation of the analytical expression, the following assumptions are made:

- Dominant background gas of neutrals
- Uniform pressure
- Constant temperature
- Constant rate coefficient for ionization
- No external electric field
5.2 Validation

- Rotational symmetry
- Uniform B field in the axial direction

The assumptions of a dominant background gas and uniform pressure and temperature imply that effectively, the electrons and ions only collide with the background gas. The friction due to these collisions is uniform over the plasma, because the number density of the background gas is uniform. When no electric field is present, this leads to a uniform ambipolar diffusion coefficient as derived in section 4.4. However, this ambipolar diffusion coefficient does depend on the magnetic field strength.

Assuming rotational symmetry, the particle balance for the electrons in cylindrical coordinates can be written as:

\[
-\frac{1}{r} \frac{\partial}{\partial r} D_a r \frac{\partial n_e}{\partial r} = n_e n_0 K, \tag{5.6}
\]

where \(D_a\) is the ambipolar diffusion coefficient derived in section 4.4, \(n_0\) the density of the background species and \(K\) the rate coefficient for ionization. Since the temperature and pressure are constant and there is a dominant background gas, the ambipolar diffusion coefficient \(D_a\) is constant. Therefore, the electron balance can be written as:

\[
\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial n_e}{\partial r} = -\frac{n_e n_0 K}{D_a}. \tag{5.7}
\]

Introducing the spatial frequency \(k = \sqrt{n_0 K / D_a}\) and the dimensionless variable \(x = kr\), the equation becomes:

\[
x^2 \frac{\partial^2 n_e}{\partial x^2} + x \frac{\partial n_e}{\partial x} + x^2 n_e = 0. \tag{5.8}
\]

The solution to this equation is a linear combination of Bessel functions of the first and second kind:

\[
n_e = AJ_0(x) + BY_0(x), \tag{5.9}
\]

with \(A\) and \(B\) constants to be determined from the boundary conditions. The boundary conditions that are used are:

\[
\frac{\partial n_e}{\partial x} \bigg|_{x=0} = 0, \quad n_e(x_b) = n_b, \tag{5.10}
\]

where \(x_b\) is the dimensionless position of the boundary. The coefficient \(B\) must be zero, since the Bessel function of the second kind is unbounded in the origin. Application of the boundary conditions gives the final expression for the electron density:

\[
n_e = n_b \frac{J_0(x)}{J_0(x_b)} \tag{5.11}
\]
Test model The model consists of a cylindrical domain. A magnetic field is applied along the axis. At the top and the bottom of the cylinder, Neumann boundary conditions are applied for all variables, thereby making the simulation quasi one dimensional. The model was run for different values of the magnetic field varying from 0 to 5 Tesla, with $T_e = T_h = 1000$ K and a constant rate coefficient of $K = 5 \cdot 10^{-22}\text{s}^{-1}$.

The pressure was 10000 Pa and the electron density at the wall of the cylinder was set to $10^{13}\text{m}^{-3}$. Note that the conditions in this plasma are chosen such, that the assumptions mentioned earlier in this section are fulfilled. The purpose of the model is to validate the implementation of the self consistent diffusion equations, not to represent a physically relevant plasma. The results of the model can be seen in figure 5.1. As expected, the electron density increases with increasing magnetic field. With increasing magnetic field the diffusion coefficient becomes smaller. Due to the smaller diffusion coefficient the losses to the wall are smaller and the electron density becomes higher.

The results from the model were fitted with equation 5.11 to obtain the ambipolar diffusion coefficient. This diffusion coefficient was plotted as a function of the Hall parameter, which can be seen in figure 5.2. The Hall parameter is defined as:

$$H = \frac{\omega_e \tau_e}{4},$$

where $\omega_e$ is the Larmor frequency of the electron and $\tau_e$ the collision time of
5.2 Validation

Figure 5.2: Ambipolar diffusion coefficient as a function of the Hall parameter. Note the logarithmic scale on the x-axis and the y-axis. The dotted lines give the asymptotic behavior of the ambipolar diffusion coefficient. When the Hall parameter is very small, the ambipolar diffusion coefficient is constant, when the Hall parameter is much larger than unity, the ambipolar diffusion coefficient scales as $1/H^2$.

the electron. For small Hall parameters, the diffusion coefficient is approximately constant, which is the expected result since the electrons are not magnetized when the Hall parameter is small. For large values of the Hall parameter, it is expected that the ambipolar diffusion coefficient scales with $1/H^2$ (equation 4.42). As can be seen from figure 5.2 this is indeed the case.
Chapter 6

Calculation of the flow field in Plasimo

6.1 Introduction

An important aspect of a plasma model is the bulk motion of the plasma. For calculation of this bulk motion, methods from computational fluid dynamics are used. In fluid dynamics, a distinction is made between compressible and incompressible flows. In a compressible flow, the mass density changes due to changes in pressure, whereas in incompressible flows this is not the case. Due to this difference, the solution strategies for compressible and incompressible flows are also slightly different.

In this chapter the solution procedure for flow calculation in Plasimo will be discussed. Section 6.2 will start with explaining the SIMPLE algorithm, which is the algorithm Plasimo uses for calculation of the flow field. This is an algorithm that can solve an incompressible or slightly compressible flow field. For highly compressible flows the SIMPLE algorithm can be extended with Karki corrections [22]. Karki corrections will be discussed in section 6.3. Besides the bulk motion, the chemical composition of the plasma is also calculated in Plasimo. This chemical mixture calculation appears to have consequences for the flow calculation via the mass density. The relation between flow and mixture calculation and the consequences for solving the bulk flow will be described in section 6.4.
6.2 The SIMPLE algorithm for incompressible flows

To solve an incompressible flow field, the solution of both the momentum and continuity equation (2.1 and 2.2) has to be found. The difficulty in solving these two equations simultaneously is the fact that in the momentum equation the pressure gradient acts as a source term. This pressure is not known, because it is one of the parameters that must be solved. The solution to this problem is given by the continuity equation. Implicitly, the correct pressure is provided by the continuity equation: if the correct pressure is substituted in the momentum equation, the resulting velocity field should satisfy the continuity equation. The indirect information in the continuity equation must thus be converted into a direct algorithm for the calculation of the pressure to solve the flow field.

The algorithm that is used for this in Plasimo is the SIMPLE algorithm: Semi Implicit Method for Pressure Linked Equations [29, 39]. There are a number of solution strategies which are closely related to the SIMPLE algorithm, amongst others SIMPLER, SIMPLEC and PISO [39]. Since these are all variations based on the same idea, and the SIMPLE algorithm is the algorithm actually used in Plasimo, the explanation in this chapter is restricted to the SIMPLE algorithm.

The explanation of the SIMPLE algorithm in this chapter will proceed along the same lines as [29]. The algorithm starts with guessing a pressure $p^*$. This pressure can be put in the discretized momentum equations, after which the velocity field can be calculated. In general, the velocity field $v^*$ calculated from this initial guess $p^*$ will not satisfy the continuity equation. The next step in the SIMPLE algorithm is to find a correction $p'$ to the guessed pressure $p^*$, such that the resulting velocity field will satisfy the continuity equation.

Assume that the correct pressure is given by:

$$p = p^* + p', \quad (6.1)$$

where $p'$ is the pressure correction. Due to the pressure correction the velocities will also change:

$$u = u^* + u', \quad v = v^* + v', \quad w = w^* + w'. \quad (6.2)$$

The question is how to calculate the pressure correction $p'$ and how to use this pressure correction to calculate the velocity corrections. Therefore, the
continuity and momentum equations are discretized. The relation between the pressure and the velocity correction will follow from the discretized momentum equation, the pressure correction is calculated from the discretized continuity equation.

Figure 6.1: Staggered control volumes for the discretization of the momentum equation for deriving the discretized equations for $p'$ and $u'$. Note that for calculation of $v^*$ from $p^*$ the momentum equation is discretized on a colocated grid. The dark grey rectangle indicates the control volume for discretization in the north-south direction, the light grey rectangle indicates the control volume for discretization in the east-west direction.

Plasimo uses the control volume method for discretization. In figure 6.1 the Plasimo grid and the control volumes for discretization of the momentum equations for determining the response of $u'$ on $p'$ can be seen. The SIMPLE algorithm is often used in combination with a staggered grid [29, 39], but Plasimo uses a colocated grid. In a colocated grid, velocities are defined on the nodal points. However, for derivation of the pressure correction equation in Plasimo, the staggered grid of Patankar [29] is used. As a result, in the discretized pressure correction equation, terms containing the velocity $v^*$ defined on the nodal boundaries occur. Since this velocity $v^*$ is in Plasimo calculated on a colocated grid, a special interpolation scheme is needed. This interpolation scheme is discussed in [25] and [36].
In the following, it is assumed that the flow problem is two dimensional and that there is no time dependency. Integrating equation 2.2 over the control volume gives the following result for the east-west direction:

\[ a_e u_e = \sum a_{nb} u_{nb} + b_{ew} + (p_P - p_E) A_e, \]  

(6.3)

where \( a_e = (\rho u_e) \Delta y \), \( A_e = \Delta y \) and \( b_{ew} \) contains the forces in the east-west direction that are not related to the pressure gradient. In this discretization the mass density is assumed to be constant. When dealing with a compressible flow the effect of the mass density must be included. How this is done will be discussed in the next section. The velocity can be solved from the momentum equation if the pressure field is given or estimated. Assume that the pressure is guessed by \( p = p^* \), the resulting velocity \( u^* \) will then follow from:

\[ a_e u_e^* = \sum a_{nb} u_{nb}^* + b_{ew} + (p_P^* - p_E^*) A_e. \]  

(6.4)

Unless \( p^* \) is the correct pressure, the resulting velocity field will not satisfy the continuity equation. By subtracting 6.4 from 6.3, the following is obtained:

\[ a_e u_e' = \sum a_{nb} u_{nb}' + (p_P' - p_E') A_e. \]  

(6.5)

As is pointed out in [29], it is possible to leave out the term \( \sum a_{nb} u_{nb}' \). The response of the velocity correction on the pressure correction becomes:

\[ u_e' = \frac{A_e}{a_e} (p_P' - p_E') = d_e (p_P' - p_E'). \]  

(6.6)

This equation shows how the guessed velocity is to be corrected in response to the pressure correction. Now the pressure correction has to be found, such that the resulting velocity field will satisfy the continuity equation. This is done by discretizing the mass continuity equation. Integration over the control volume in figure 6.2, leads to the following expression:

\[ [(\rho u)_e - (\rho u)_w] \Delta y + [(\rho v)_n - (\rho v)_s] \Delta x = 0 \]  

(6.7)

substituting of the relations between the velocity and pressure correction:

\[ u_e = u_e^* + d_e (p_P' - p_E') \]
\[ u_w = u_w^* + d_w (p_W' - p_P') \]
\[ v_n = v_n^* + d_n (p_P' - p_N') \]
\[ v_s = v_s^* + d_s (p_S' - p_P') \],
6.2 The SIMPLE algorithm for incompressible flows

gives the discretization equation for $p'$:

$$a_P p'_P = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + b,$$

(6.8)

where $a_P = a_E + a_W + a_N + a_S$, with $a_E = \rho_e d_e \Delta y$ (other directions are similar) and $b = [(\rho u^*_w - (\rho u^*)_e] \Delta y + [(\rho v^*_s - (\rho v^*)_n] \Delta x$.

![Control volume for discretization of the continuity equation.](image)

For calculation of the discretization coefficients the mass density thus has to be known on the control volume boundaries. To calculate the mass density on these boundaries, an interpolation scheme is needed. In the beginning of this project, it was found that for high Mach number flows, this interpolation was not carried out correctly in Plasimo (appendix A.3). From equation 6.8, it can be seen that $b$, which is the mismatch from the continuity equation, acts as a source term. If the starred velocities $v^*$ fulfill continuity, the $b$ term in the RHS of 6.8 will be zero and no pressure correction is needed: the solution of the flow problem has converged. The SIMPLE solution algorithm for incompressible flows can now be summarized as follows:

- Guess the pressure field $p^*$.
- Solve the momentum equations to obtain $u^*$, $v^*$.
- Solve the pressure correction equation (6.8).
- Calculate $p$ by adding the pressure correction: $p = p^* + \alpha p'$.
• Calculate the velocities with the velocity correction formulas (6.6).

• Solve the other equations that depend on the flow (temperature, mixture, transport coefficients).

• Use the corrected pressure $p$ as the new guess $p^*$ and repeat the procedure until convergence.

As can be seen, only part of the pressure correction $p'$ is added to $p^*$. This under-relaxation $\alpha$ is applied to avoid divergence as is pointed out in [29]. In calculation of $u^*$ and $v^*$ from the discretized momentum balance some under-relaxation can also be applied. The following section will discuss the changes in the solution procedure when the flow is compressible.

### 6.3 Compressible flows: Karki corrections

The procedure described in section 6.2 is used when the flow is incompressible: a change in pressure does not effect the mass density. In compressible flows a change in pressure will effect the mass density. Karki corrections take into account the influence of pressure on the mass density. Besides the velocity, the mass density is now also corrected after the pressure correction is calculated. Note that the calculation of the pressure correction also changes due to the contribution of the mass density.

For calculation of the pressure correction equation in a compressible flow, the mass flux is approximated by [29]:

$$\rho u = (\rho^* + \rho') (u^* + u') = \rho^* u^* + \rho' u^* + \rho^* u', \quad (6.9)$$

where the term $\rho' u'$ has been neglected [29]. Furthermore, the following relation between the pressure and the mass density correction is assumed:

$$\rho' = K p'. \quad (6.10)$$

The discretization of the continuity equation is now given by:

$$[(\rho^* u^*)_e - (\rho^* u^*)_w] \Delta y + [(\rho^* v^*)_n - (\rho^* v^*)_s] \Delta x +$$
$$[(\rho^* u')_e - (\rho^* u')_w] \Delta y + [(\rho^* v')_n - (\rho^* v')_s] \Delta x +$$
$$[(\rho' u^*)_e - (\rho' u^*)_w] \Delta y + [(\rho' v^*)_n - (\rho' v^*)_s] \Delta x = 0 \quad (6.11)$$

Substituting relations 6.10 and 6.6 gives:

$$[(\rho^* u^*)_e - (\rho^* u^*)_w] \Delta y + [(\rho^* v^*)_n - (\rho^* v^*)_s] \Delta x +$$
6.3 Compressible flows: Karki corrections

\[
\begin{align*}
\left[ (\rho^* d_e (p'_p - p'_E))_e - (\rho^* d_w (p'_W - p'_P))_w \right] \Delta y + \\
\left[ (\rho^* d_n (p'_p - p'_N))_n - (\rho^* d_s (p'_S - p'_P))_s \right] \Delta x + \\
\left[ (K_e (p'_p - p'_E) u^*)_e - (K_w (p'_W - p'_P) u^*)_w \right] \Delta y + \\
\left[ (K_n (p'_p - p'_N) v^*)_n - (K_s (p'_S - p'_P) v^*)_s \right] \Delta x = 0
\end{align*}
\] (6.12)

This can be rearranged to the same form as equation 6.8, where the discretization coefficients are given by

\[
a_P = a_E + a_W + a_N + a_S,
\] (6.13)

with

\[
a_E = (\rho_e^* d_e + K_e u^*) \Delta y.
\] (6.14)

The coefficients \(a_W, a_N, a_S\) are calculated in a similar way. As can be seen, Karki corrections correct the mass density. But Karki corrections also change the equation from which the pressure correction is calculated. The particular form of the Karki correction does not influence the final solution, but it influences the convergence path towards the solution. A bad choice for the Karki correction can therefore lead to divergence. Changes made to the choice for \(K\) are discussed in appendix A.2. In principle, in a compressible flow/plasma model the density can also be calculated from an equation of state. However, when the flow is strongly compressible Karki corrections may be necessary [29]. In Plasimo the equation of state (ideal gas law) is used in plasma models to couple the flow pressure to the species densities of the chemistry calculation. The consequences of this coupling and Karki corrections for the flow calculations will be discussed in the following section.

**Underrelaxation** As explained in 6.2, the momentum equation from which \(v^*\) is determined can be under-relaxed for stability reasons. The pressure correction may be under-relaxed as well, by adding only a part of the pressure correction \(p'\) to the pressure. It was found that in Plasimo, the discretization coefficients of the pressure correction equation were also partly under-relaxed. This caused large deviations from continuity during the iteration process and often led to divergence. This problem has been solved now, as explained in appendix A.1. In Plasimo, one can choose to under-relax the Karki correction with an under-relaxation factor \(\beta\):

\[
\rho' = \beta \ast K p' \quad u' = d p'.
\] (6.15)

This under-relaxation has no consequences for mass continuity, but makes the mass density correction relatively less important to the velocity correction.
6.4 Interaction of flow and chemistry

In a plasma model not only the flow, but other plasma parameters like electron and heavy particle temperature and transport coefficients are calculated as well. In chapter 2 the iteration scheme for a complete nLTE plasma model was presented. After the flow calculation, chemical composition and electron and heavy particle temperature are calculated. The chemical composition calculation determines absolute species densities. In general, during iteration, the absolute species densities together with the temperature will not give the pressure as calculated by the flow calculation:

\[ p \neq \sum_i n_i k T_i \]  \hspace{1cm} (6.16)

In Plasimo, there are two possibilities to adapt the species densities to match the total pressure: particle 0 and scaling [14]. In the first method, the density of one species (particle 0) is adapted such that summation over the partial pressures yields the total pressure. In the second method, all the species are scaled with the same factor per grid cell to match the total pressure. Since these two methods alter the densities they can be seen as a mass density changing mechanism. Therefore, applying Karki correction in a plasma model may not be necessary, since this matching of species densities and pressure already acts as an equation of state. However, besides acting as a mass density changing mechanism, Karki corrections also change the velocity correction (6.3). The higher the Mach number, the weaker the coupling between the pressure and the velocity correction. Not applying Karki corrections at high Mach number flows can lead to divergence. On the other hand, applying Karki corrections, while simultaneously calculating the chemical composition, can give rise to a slower convergence speed. Sometimes, it can even lead to divergence. This competition between positive and negative aspects of Karki corrections will be demonstrated with the convergence behavior of a plasma model, that includes both flow and composition calculation.

Model description and results  A schematic picture of the model that was used to study the interaction between flow and chemistry can be seen in figure 6.3. At the inlet and the outlet the pressure is prescribed. Species present in this model are: Ar, Ar\(^+\) and electrons. At the inlet the species fractions are prescribed: Ar:Ar\(^+\):e=2:1:1. At the other boundaries the derivative of the species densities normal to the boundary was set to zero. No chemical reactions are present in the model. The model was run for three
values of the outlet pressure: 3990 Pa (incompressible flow), 3900 Pa (compressible) and 2500 Pa (highly compressible). The inlet pressure was fixed at 4000 Pa. The other boundary conditions for the flow field can be seen in table 6.1. For each value of the outlet pressure, the model was run with both the scaling and particle 0 method to match the species densities with the pressure. A fixed temperature of 5000 K for both the electrons and the ions is prescribed. The under-relaxation factor of the Karki corrections was also varied.

The results of the model can be seen in figure 6.4. As can be seen, in the compressible and highly compressible flow the number of iterations increases as function of the Karki under-relaxation factor, while for incompressible
flows the number of iterations remains constant. This negative influence of
the Karki corrections on the convergence behavior is probably due to the fact
that the mass density itself is not corrected. After the pressure correction
has been calculated, the massflux \( \rho v \) is corrected via:

\[
\rho v = \rho^* v^* + v^* Kp' + \rho^* dp',
\]

(6.17)

and the velocity via:

\[
v = v^* + dp'.
\]

(6.18)

As can be seen in the iteration scheme in chapter 2, after the velocity, the
composition is calculated. This is done via equation 2.3. However, the bulk
velocity needed in this equation, is in Plasimo calculated as the massflux
divided by the mass density:

\[
u = \frac{\rho u}{\rho},
\]

(6.19)

which does not yield the bulk velocity, since \( \rho \) is not corrected by Karki
corrections.
Figure 6.4: Number of iterations as function of the Karki under-relaxation factor. The strongly compressible flow corresponds with an outlet pressure of 2500 Pa, the compressible flow to an outlet pressure of 3900 Pa and the incompressible flow to an outlet pressure of 3990 Pa. The highly compressible flow does not converge without applying Karki corrections. Note that the absolute number of iterations can not be compared between the flow types (incompressible-compressible-highly compressible) since between these flow types other under-relaxation factors differ as well.
Chapter 7

Simulation of shock waves

7.1 Introduction

As described in chapter 1, both Magnum and Pilot PSI consist of a cascaded arc plasma source and a vacuum vessel into which the plasma expands supersonically. Beside the Magnum and Pilot experiment, supersonic plasma jets occur in industrial plasma applications like low pressure plasma spraying (LPPS), thermal plasma chemical vapor deposition (TPCDV) and plasma preparation of nanosized powders [32]. In astrophysical plasmas shockwaves can be encountered as well. It is therefore of interest to study shockwaves in depth.

Due to the large hydrodynamic velocities in a supersonic jet, fluid dynamic time scales can exceed the chemical kinetic timescales of interest [16]. In this situation, the plasma is not in local thermodynamic equilibrium, and nLTE modeling becomes necessary. There have been a number of numerical studies on expanding plasma jets, see for example [3, 6, 7, 10, 12, 16, 32, 38]. In these studies different approaches of modeling of the plasma jet are used. Most studies simplify the plasma by only modeling the neutrals [10, 38], assuming LTE [12, 32] or using an MHD approach [10, 12]. Some studies include chemistry [3, 6, 7, 16], however none of the nLTE models are concerned with magnetized plasmas.

For the modeling of Magnum PSI an nLTE approach that can handle supersonic, magnetized plasma is needed. In this chapter, the ability of Plasimo to handle supersonic jets is demonstrated. To this end, simulations of an overexpanded and underexpanded jet have been carried out.
This chapter is organized as follows, in section 7.2 the typical properties of overexpanded and underexpanded jets are discussed. In section 7.3, it is shown that with the SIMPLE algorithm presented in chapter 6 together with recent changes in the flow code (appendix A) these jets can be simulated. However, simulations presented in this chapter are carried out with a uniform composition over the plasma. When more complex chemistry is added, problems arise, especially in the presence of temperature gradients. This problem and the assumptions made in the model are discussed in section 7.4.

7.2 Over- and underexpanded plasma

The flow of plasma expanding from a nozzle into a vacuum chamber can be fully expanded, overexpanded or underexpanded [8, 11]. If the pressure at the outlet of the nozzle is lower than the chamber pressure, the flow is overexpanded. If the pressure at the outlet of the nozzle is higher than the pressure of the vacuum chamber, the flow is underexpanded. Both underexpanded and overexpanded flows show one or more shock waves. These shockwaves equalize the jet pressure with the background pressure.

Overexpansion In an overexpanded jet, the background pressure is higher than the pressure of the jet leaving the nozzle. In figure 7.1, an overexpanded jet can be seen. Because of the higher background pressure, the jet is squeezed inward when leaving the nozzle (2). This compression increases

![Figure 7.1: Shock wave structures in an overexpanded jet. (1: High pressure reservoir, 2: Nozzle exit, 3: Oblique shock waves, 4: Mach disk, 5: Expansion fan, 6: Free jet boundary, 7: Compression fan, 8: Shock triple point)](image)

the pressure in the jet. The squeezing of the jet and the pressure increase is made possible by oblique shock waves (3). Oblique shockwaves are shockwaves which are inclined with respect to the flow direction [11]. By passing the normal shock wave or Mach disk (4), which is oriented perpendicular to the flow direction [11], the pressure in the jet is also increased. However,
the flow may be compressed so much that its pressure now exceeds the background pressure. The flow then expands outward in the presence of expansion waves (5) to reduce the pressure again. These expansion waves reflect from the jet boundary (6), forming compression waves (7). These compression waves can merge, creating an oblique shockwave, after which the cycle of compression and expansion starts over again.

The difference between jet and background pressure becomes smaller with each compression-expansion cycle. This damping is due to viscous dissipation, which occurs when the expansion fan reflects from the jet boundary. The area outside the jet boundary is called the zone of silence.

**Underexpansion** In an underexpanded jet, the background pressure is lower than the jet pressure, causing the jet to expand beyond the nozzle. This can be seen in figure 7.2. The subsequent compression and expansion events are the same in the overexpanded and underexpanded jet. The only difference is that the overexpanded jet starts with a compression whereas the underexpanded jet starts with an expansion.

![Figure 7.2: Shock wave structures in an underexpanded jet. (1: High pressure reservoir, 2: Nozzle exit, 3: Oblique shock waves, 4: Mach disk, 5: Expansion fan, 6: Free jet boundary, 7: Compression fan, 8: Shock triple point)](image_url)

7.3 Shock wave model and results

The shock wave model consists of a cylindrical geometry, which can be seen in figure 7.3. At the inlet, the plasma flows into the vessel. By varying the boundary conditions for the pressure at the wall and the inlet, the flow can be chosen to be overexpanded or underexpanded. In table 7.1 the settings of the model for the overexpanded and underexpanded calculation can be seen. When simulating shockwaves, the grid must be fine enough to resolve these shockwaves. For the model, a computational grid was used with 112 cells in
the axial direction and 160 cells in the radial direction. In figure 7.4, the grid is schematically depicted. As can be seen in table 7.1, the geometry of the overexpanded flow has smaller physical dimensions than the underexpanded flow. The reason for this is that the overexpanded jet is compressed when leaving the nozzle, leading to smaller structures in the jet. To be able to resolve these smaller structures with the same number of grid cells, smaller physical dimensions are taken.

For the composition calculation, an nLTE model is used. The species taken into account are Ar, Ar$^+$ and electrons. An ionization degree of 1 % is prescribed, chemical reactions are not taken into account.

In figure 7.5, the simulated Mach number of both the underexpanded and overexpanded jet can be seen. In the overexpanded jet the Mach number is highest just outside the inlet, the maximum of the underexpanded jet Mach number is found further into the plasma. In both jets, the zone of silence can be seen as the area without contours.
Figure 7.4: Computational grid for the underexpanded flow. The grid for the overexpanded flow has different physical dimensions, but the same amount of grid cells and stretching. For clarity, the grid in this figure has 28 cells in the axial and 40 cells in the radial direction. The real grid has 112 x 160 cells.

In figure 7.6 and 7.7, the axial and radial velocity can be seen respectively. From these figures it can be seen that Plasimo is able to capture the typical multiple shock wave structure as present in overexpanded and underexpanded flow. Especially in the radial velocity of the overexpanded flow the reflections from the jet boundary are clear, as the radial velocity changes sign with each reflection. When compared to for example [10], the shock wave structures damp out quickly. This difference can be explained by the fact that the plasma model presented here consists of 1% ions leading to a high viscosity, whereas [10] uses neutral gas and Euler equations. The results of [10] can not be reproduced with Plasimo, since Plasimo is only capable of solving laminar flow.

The difference between overexpanded and underexpanded flow can also clearly been seen in figures 7.8 and 7.9. The temperature in the overexpanded jet increases with respect to the inlet temperature due to compression, whereas the underexpanded jet decreases in temperature due to expansion. In both simulations, the viscous dissipation near strong velocity gradients can be seen. Only the heavy particles receive this heat from viscous dissipation, since the electrons do not carry viscosity.
Figure 7.5: Mach number in overexpanded and underexpanded flow.
Figure 7.6: Axial velocity in overexpanded and underexpanded flow. The underexpanded jet expands beyond the nozzle, while the overexpanded jet is squeezed inward.
Simulation of shock waves

Figure 7.7: Radial velocity in overexpanded and underexpanded flow.
Figure 7.8: Heavy particle temperature in overexpanded and underexpanded flow.
Figure 7.9: Electron temperature in overexpanded and underexpanded flow.
7.4 Discussion

With the simulations in this chapter it has been shown that with the recent changes in the flow code, Plasimo is able to simulate the flow in the expansion region of Magnum PSI. Specific properties of supersonic jets, such as the multiple shockwave structure can be captured. In this section, the possibility of adding a composition calculation to the flow model is commented on. Furthermore, assumptions regarding laminarity, grid size and fluid equations are discussed.

Chemistry In this chapter, variation of the composition over the plasma was not considered. One of the interests of the Magnum PSI project is the influence of the capturing of neutrals in the plasma beam. Also the behavior of the jet in a magnetic field is a research topic. For both studies, a composition calculation, including the diffusive transport is needed. Attempts to expand the model to include this, led to divergence and violation of species conservation. Especially near the wall, and in regions with strong temperature gradients, problems arose. For this reason, a simple test model was set up to analyze the problem. The test model and results of the model will be discussed in chapter 8.

Laminar flow In Plasimo, it is assumed that the simulated flow is laminar. Since the simulated supersonic jets in this chapter have a high velocity, this assumption must be justified. To investigate whether the flow is laminar or turbulent, the Reynolds number of both the underexpanded and overexpanded jet will be calculated. The Reynolds number gives the ratio between inertial and viscous forces and is defined as:

\[ Re = \frac{UL}{\nu}, \quad (7.1) \]

where \( U \) is the typical velocity of the flow, \( L \) is the typical length scale of the flow and \( \nu \) the kinematic viscosity. The kinematic viscosity is related to the dynamic viscosity \( \mu \) and the mass density \( \rho \) via:

\[ \nu = \frac{\mu}{\rho}, \quad (7.2) \]

For the typical length scale in the flow, the radius of the vacuum vessel or the radius of the plasma jet can be chosen. The plasma jet radius is the most logical choice, since outside the jet, in the zone of silence, the flow velocity is zero. In table 7.2, viscosity, density, length scale and Reynolds number are listed for the overexpanded and underexpanded jet simulated in this chapter.
Simulation of shock waves

<table>
<thead>
<tr>
<th></th>
<th>Underexpanded</th>
<th>Overexpanded</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic viscosity</td>
<td>$10^{-4}$ Pa · s</td>
<td>$10^{-3}$ Pa · s</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>$10^{-1}$ m$^2$/s</td>
<td>$10^{-1}$ m$^2$/s</td>
</tr>
<tr>
<td>Jet radius</td>
<td>0.005 m</td>
<td>0.005 m</td>
</tr>
<tr>
<td>Density</td>
<td>$10^{-3}$ kg/m$^3$</td>
<td>$10^{-2}$ kg/m$^3$</td>
</tr>
<tr>
<td>Velocity</td>
<td>5000 m/s</td>
<td>10000 m/s</td>
</tr>
<tr>
<td>$Re_{jet}$</td>
<td>250</td>
<td>500</td>
</tr>
</tbody>
</table>

Table 7.2: Reynolds number for the overexpanded and underexpanded jet.

As can be seen in the table, both for the overexpanded and underexpanded jet, the Reynolds number is below 2000. Although this value of 2000 is not a strict criterion to determine whether the flow is turbulent, it is reasonable to assume that the jets are laminar. It seems remarkable that supersonic flow can be laminar. This is possible, due to the very high viscosity in a plasma, which is caused by the high temperatures and charged particle interactions. This very high viscosity could also been seen in the rapid damping of the shock wave structures in this chapter as compared to simulations of [10].

**Grid size**  In the results presented in this chapter large gradients in velocity, temperature etc. occurred due to shock waves. When such sharp gradients are present, it is necessary to test whether the grid is fine enough to capture all features of the flow. This testing is done by doubling the

Figure 7.10: On axis pressure and heavy particle temperature for the underexpanded flow for different number of grid points.
number of grid points in both directions and looking at the outcome of the model. The results can be seen in figure 7.10. For the pressure, increasing the number of grid cells gives no visible change in the outcome of the model. In the heavy particle temperature it can be seen that the coarse grid slightly underestimates the strength of the first shock. Despite this small error, it can be concluded that the coarse grid is still fine enough to give a reasonable outcome of the model.

**Fluid assumption**  In this chapter relatively high pressures were used for the simulation. In the vacuum vessel of Magnum PSI, the pressure will be in the order of a few Pascal. Since fluid equations are used, it is necessary to check whether these can be used at such low pressures. This can be done by investigating the Knudsen number of the plasma, which is defined as [20]:

$$Kn = \frac{\lambda}{L} = \frac{k_B T}{\sigma p L},$$  

(7.3)

where $T$ is the temperature, $\sigma$ the cross section and $p$ the pressure. The Knudsen number gives the ratio between the mean free path $\lambda$ and a typical length scale $L$. Assume that the temperature is 20000 K and the typical dimension of the vacuum vessel is 0.5 m. Substituting the momentum transfer cross-section from [30] for Ar-Ar$^+$ in equation 7.3 leads to $Kn \simeq 0.5$. Using the momentum transfer cross-section for H$^+$-H$_2$ from [31] gives $Kn \simeq 5$. To describe the neutrals accurately a statistical method should be used, since the Knudsen number is rather large. However, it can be argued that a fluid approach can still give a reasonable estimate, especially since the temperature of the neutrals will probably be smaller than 20000 K. For the ions a fluid approach can be used definitely, since their mean free path will be much smaller than calculated here due to the magnetic field.
Simulation of shock waves
Chapter 8
Multi-component plasmas

When modeling a multi-component flowing plasma such as Magnum PSI, the bulk motion of the plasma as well as the motion of the different components has to be described. As described in chapter 2, in Plasimo, the bulk flow is found by means of a combined solution of the continuity (2.1) and Navier Stokes (2.2) equation, while the distribution of the different species in the bulk is calculated by the species balance (2.3). To solve the species balance, an expression for the diffusive velocity is needed, which was given in chapter 4. When modeling multi-component plasmas in Plasimo it is often difficult to get convergence. Sometimes converged results are not physical, especially in the presence of temperature gradients. This chapter is an attempt to analyse the problems with the help of a very simple test model. First, the discretization of the species balance is discussed in section 8.1. In section 8.2 the simple test model and results from the test model are presented. The last section gives a discussion on the results.

8.1 Discretization of the species balance

In Plasimo, the equations presented in chapter 2, are cast in the general form of the so-called \( \phi \) equation [18, 21]:

\[
\nabla \cdot (U \phi) - \nabla \cdot (\Gamma \nabla \phi) = S_c + S_p \phi
\]

(8.1)

In the case of the species balance, the number density \( n \) is the \( \phi \) variable. The convection term is given by \( U \), while \( \Gamma \) describes the diffusion term. Chemical reactions are described by the source terms \( S_c \) and \( S_p \).
The \( \phi \) equation in Plasimo is discretized on a control volume grid, see figure 8.1. Integration of the \( \phi \) equation over a control volume in the absence of source terms gives the discretized species balance [18, 29]:

\[
a_P \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S,
\]

(8.2)

where the discretization coefficients are given by:

\[
\begin{align*}
a_E &= D_e A(|P_e|) + [-F_e, 0] \\
a_W &= D_w A(|P_w|) + [F_w, 0] \\
a_N &= D_n A(|P_n|) + [-F_n, 0] \\
a_S &= D_s A(|P_s|) + [F_s, 0] \\
a_P &= a_E + a_W + a_N + a_S + F_e - F_w + F_n - F_s,
\end{align*}
\]

with the conductances defined as:

\[
D_e = \frac{\Gamma_e \Delta y}{\delta x_e}, \quad D_w = \frac{\Gamma_w \Delta y}{\delta x_w}, \quad D_n = \frac{\Gamma_n \Delta x}{\delta y_n}, \quad D_s = \frac{\Gamma_s \Delta x}{\delta y_s},
\]

and the flow rates as:

\[
F_e = (\rho u)_e \Delta y, \quad F_w = (\rho u)_w \Delta y, \quad F_n = (\rho u)_n \Delta x, \quad F_s = (\rho u)_s \Delta x.
\]

The brackets [] denote the maximum value of the arguments inside the brackets. The function \( A \) is dependent on the discretization scheme used, in Plasimo a hybrid discretization scheme is used, which gives:

\[
A(|P|) = [0, 1 - 0.5|P|], \quad (8.3)
\]
8.2 The two types of argon model

with $P$ the Peclet number which is defined as:

$$P = \frac{F}{D}. \quad (8.4)$$

This numerical Peclet number gives the ratio between the convection and diffusion terms in the $\phi$ equation.

As explained in chapter 5, the calculated diffusion velocity is split into a convective and a diffusive part following:

$$\mathbf{v}_i^* = \mathbf{v}_i + \frac{D_i}{n_i} \nabla n_i. \quad (8.5)$$

The term $\mathbf{u} + \mathbf{v}_i^*$ is put into the convective part $\mathbf{U}$ of the $\phi$ equation, $D_i$ is put into the diffusive part $\Gamma$. This has the consequence, that the numerical Peclet number does not give the ratio between the physical quantities of convection and diffusion.

It is important to note that the term $F_e - F_w + F_n - F_s$ in the discretization coefficient $a_p$ is zero when the flow field is divergence free [29, 39]. If only the bulk velocity is used in the convection term, this condition is automatically fulfilled since the bulk flow field is divergence free. However if $\mathbf{u} + \mathbf{v}_i^*$ is used in the convection term, $F_e - F_w + F_n - F_s$ is in general not zero. Both Patankar [29] and Versteeg [39], mention a divergence free convection term as an important property of a discretization scheme. The consequences of violation of this property will be discussed in more detail in section 8.3.

8.2 The two types of argon model

To get more insight in the problems with the chemistry calculation, a test model was set up. This model describes the flow of 'two types of argon' in a cylindrical geometry. In figure 8.2 a schematic picture of the model can be seen. At both the inlet and the outlet, the pressure is described. By varying the difference between inlet and outlet pressure, the flow velocity can be controlled. The boundary conditions for the flow variables can be seen in table 8.1. In the model there are two species: Ar1 and Ar2, with exactly the same properties. At the inlet the density for both Ar1 and Ar2 is set to 0.5 times the total species number density, on the other boundaries the density gradients are calculated following [18]. The diffusion velocity $\mathbf{v}_i$ is calculated with self consistent diffusion approach as described in [18]. This approach is very similar to the approach described in chapter 4, but without
Multi-component plasmas

a magnetic field. There are no chemical reactions in the model. The Ar2 density is calculated with the $\phi$ equation. For calculation of the $D_i$ used for splitting of the diffusion velocity is calculated as [18, 21]:

$$D_i = \left( \sum_{j \neq i} \frac{z_j}{D_{ij}} \right)^{-1}, \quad D_{ij} = \frac{p_ip_j}{p_if_{ij}} \quad (8.6)$$

with $z_j = p_j/p$ and $f_{ij}$ the friction as defined in chapter 4. In the rest of this chapter this $D_i$ is referred to as the 'normal' diffusion coefficient. The Ar1 density follows from the ideal gas law. A fixed temperature profile is prescribed.

Figure 8.2: Geometry of the two types of Argon model. At the inlet, equal amounts of Ar1 and Ar2 are prescribed.

<table>
<thead>
<tr>
<th></th>
<th>Inlet</th>
<th>Outlet</th>
<th>Wall</th>
<th>Symm.axis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial velocity</td>
<td>$\frac{\partial v_z}{\partial z} = 0$</td>
<td>$\frac{\partial^2 v_z}{\partial z^2} = 0$</td>
<td>$v_z = 0$</td>
<td>$\frac{\partial v_z}{\partial r} = 0$</td>
</tr>
<tr>
<td>Radial velocity</td>
<td>$v_r = 0$</td>
<td>$\frac{\partial v_r}{\partial z} = 0$</td>
<td>$v_r = 0$</td>
<td>$v_r = 0$</td>
</tr>
<tr>
<td>Pressure</td>
<td>$p = p_{in}$</td>
<td>$p = p_{out}$</td>
<td>$\frac{\partial^2 p}{\partial r^2} = 0$</td>
<td>$\frac{\partial p}{\partial z} = 0$</td>
</tr>
</tbody>
</table>

Table 8.1: Boundary conditions of the two types of argon model.

The expected result of the test model is an equal partial pressure for both Ar1 and Ar2. Furthermore, there should be conservation of species, since there are no chemical reactions in the model. As will be shown, in the
8.2 The two types of argon model

presence of temperature gradients, Plasimo does not give the expected result. It was found that species conservation was not satisfied, whereas overall mass conservation was satisfied. In the following paragraphs, the influence of grid size, temperature gradient, diffusion coefficient and flow velocity on the model outcome are studied.

The influence of grid size  The two types of argon model was run with a fixed temperature profile (in Kelvin) of \( T = 1000 + 1000z/z_{max} \). The inlet pressure was 31000 Pa, the outlet pressure was 30000 Pa. The number of grid points in the model was varied. Figure 8.3 shows the on-axis profile of

![Graph showing dependence on grid size](image)

Figure 8.3: Dependence of the model on the grid size. RP stands for Refinement Power, the number of gridpoints in a model is: \((2^{RP} \times 16) \times (2^{RP} \times 16)\). The figure shows the on-axis partial pressures for both Ar1 and Ar2.

The partial pressures of Ar1 and Ar2. As can be seen, doubling the number of grid cells, leads to a more physical outcome of the model. This suggests that the model, consisting of equations and boundary conditions, is physically correct but that the problem is a discretization error. It can also be seen in figure 8.3, that one cell away from the inlet, the value of the Ar2 partial pressure is not bounded by the values of the neighboring cells. Boundedness is discussed in section 8.3.

The influence of the temperature gradient  The two types of argon model was also run on a coarse grid (refinement power = 0) for different temperature profiles. Again, the inlet pressure was 31000 Pa, the outlet pressure was 30000 Pa. In figure 8.4 the partial pressures of Ar1 and Ar2 can be
Figure 8.4: Dependence of the model on the temperature gradient. The on-axis partial pressures of Ar1 and Ar2 are shown. Note that for a positive temperature gradient, the calculated partial pressure for Ar2 is too low, whereas for a negative temperature gradient, the partial pressure of Ar2 is too high.

Figure 8.5: Dependence of the calculated Ar2 partial pressure on the temperature gradient. A linear temperature profile increasing from inlet to outlet is used. The inlet temperature is 1000 K for all models, the temperature difference between inlet and outlet is varied. The larger the temperature gradient, the larger the discrepancy between the expected and the actual outcome.
8.2 The two types of argon model

seen for these different temperature profiles. Without a temperature profile, the outcome is almost correct. With temperature gradients, large deviations from the expected result can be seen. If the temperature gradient changes sign, the sign of the error in the outcome of the model changes sign as well. Compare for example, the partial pressures of Ar2 for the different temperature profiles.

In figure 8.5 a linear temperature profile, increasing from inlet to outlet was used, where the temperature difference between inlet and outlet was varied. The figure shows that the larger the temperature gradient, the less correct the model outcome is.

Probably, the dependence of the error on the temperature gradient is related to the splitting of the diffusion velocity in a convective and diffusive part, which causes the numerical Peclet number to deviate from the physical Peclet number. The extent of difference between these two Peclet numbers depends on the temperature gradient, since the numerical diffusion part is $\nabla n_i$ dependent, while physically diffusion is $\nabla p_i + y_i \nabla p$ dependent.

![Figure 8.6: Dependence of the model on the flow velocity.](image)

**The influence of flow velocity**  In figure 8.6, the pressure difference between inlet and outlet was varied, thereby varying the flow velocity. The inlet pressure was 31000 Pa, the outlet pressure 30000 Pa and the model was run on a coarse grid (refinement power 0). As can be seen in figure 8.6, varying the pressure does not have a large influence on the error introduced in the
partial pressure in the first grid cell. It must be noted, however, that in all the cases the velocity is still quite large. In figure 8.7 a situation without flow can be seen. Here, the errors in the partial pressures are smaller, however still quite large for a converged result.

Figure 8.7: Partial pressures of Ar1 and Ar2 without flow. In the fixed flow run, a constant pressure and zero velocity field were prescribed. In the Delta p=0 run, a constant pressure was prescribed, but the resulting (zero) velocity field was calculated.

Figure 8.8: Dependence of the calculated Ar2 partial pressure on the diffusion coefficient. D=normal refers to $D_i$ as calculated in equation 8.6.
The influence of the diffusion contribution In figure 8.8, the diffusion coefficient $D_i$, which determines the splitting in a convective and diffusive part is varied. The inlet pressure is 31000 Pa, the outlet pressure 30000 Pa and the refinement power 0. As can be seen in the figure, variation of $D_i$ has a strong influence. This indicates that the error present in the chemistry calculation can be due to this splitting.

8.3 Discussion

In this chapter, it was found that varying grid size, temperature gradients and splitting of the diffusion velocity in a convective and a diffusive part have a large impact on the outcome of the 'two types of argon’ test model. The fact that refining the grid gives a more physical outcome, gives an indication that the problem is a discretization error and that the physical problem consisting of equations and boundary conditions is in principle well-posed. As discussed in [39], numerical results will only be physically realistic when the discretization scheme has certain fundamental properties. In this section two of these fundamental properties, the transportiveness and the boundedness, will be discussed in relation to the chemistry calculation in Plasimo. Furthermore, a possible solution to the composition calculation problem will be presented.

Transportiveness A possible reason for the discretization error is the fact that the physical Peclet number does not correspond to the numerical Peclet number. As [39] points out, it is very important that the relationship between the magnitude of the Peclet number and the directionality of influencing, known as the transportiveness, is borne out in the discretization scheme. In the composition calculation of Plasimo this is not the case, since the part of the diffusion velocity that is not dependent on $\nabla n$, but on $\nabla T$, is added to the convection term.

Boundedness Note that because of the splitting, the convection term is in general not divergence free. According to [29] and [39] a divergence free convection term is one of the requirements for proper discretization of the $\phi$ equation. This should assure that in the absence of sources, the internal nodal value of the property $\phi$ should be bounded by its boundary values. Related to this boundedness is the Scarborough criterion [39] which states that a sufficient condition for a convergent iterative method can be expressed
in terms of the values of the coefficients in the discretized equations:

\[
\sum \frac{|a_{nb}|}{|a'_P|} \begin{cases} 
\leq 1 \text{ at all nodes} \\
< 1 \text{ at one node at least}
\end{cases} \tag{8.7}
\]

where \(a'_P\) is the net coefficient of central node \(P\) \((a_P - S_P)\) and the summation is taken over all the neighboring nodes. The Scarborough criterion is automatically fulfilled when the convection term is divergence free.

**Mass fractions**  Possibly, the use of the massfraction \(y_i = \frac{n_i}{\rho}\) as a \(\phi\) variable can be a solution to the composition calculation problem. In mass fractions the \(\phi\) equation can be written as:

\[
\nabla \cdot (\rho u y_i) - \nabla \cdot (\Gamma \nabla y_i) = S_c + S_p y_i. \tag{8.8}
\]

The advantage of using mass fractions is that the temperature dependent part of the diffusion can also be put in the diffusion term of the \(\phi\) equation. However, there can still be diffusion fluxes that can not completely be fitted in \(\Gamma\). It should be examined whether it is better to put these 'remaining parts' of the diffusion flux in the source terms instead of in the convection term. This should ensure the boundedness and transportiveness of the discretization scheme.
Chapter 9

Conclusions

In this report, the use of Plasimo for modeling of the source and expansion region of Magnum PSI was explored. Special attention was paid to the question how flow, composition and temperature calculation in Plasimo should be changed to allow future modeling of Magnum PSI. Sections 9.1, 9.2 and 9.3 of this chapter draw conclusions on these questions and discuss the changes that have already been made to Plasimo.

9.1 Flow

For modeling of Magnum PSI, Plasimo should be able to calculate compressible flow fields. For this reason, adaptions have been made to the flow code (appendix A). The results of the shock wave models presented in chapter 6 demonstrate the current applicability of Plasimo for the flow calculation in the expansion region of Magnum PSI. To obtain convergence in a strongly compressible flow field, applying Karki corrections is sometimes necessary. As was shown in chapter 6, application of Karki corrections has a negative influence on the convergence behavior due to interaction with the composition calculation. By applying the Karki correction $\rho'$ to the mass density $\rho$ as well, this can easily be solved.

In a magnetized plasma, the diamagnetic current causes an extra term $\mathbf{j} \times \mathbf{B}$ in the Navier Stokes equation. Currently, this term is not taken into account in Plasimo. In the configuration of Magnum PSI, this Lorentz force term decreases the expansion of the flow in the radial direction. For an accurate description of the expansion region in the presence of a magnetic field, this term has to be included in the future. It is believed that this is possible without major changes to the code.
In Magnum PSI, the magnetic field causes anisotropy in transport coefficients, such as the viscosity. This anisotropy in the viscosity is currently not taken into account. For modeling of the source region of Magnum PSI this is probably not a big problem, since the viscosity is carried by the heavy particles, which are not magnetized in the source region. In the expansion region both electrons and ions can be magnetized and anisotropic viscosity should probably be implemented. For the implementation, the coefficients derived in chapter 3 can be used.

9.2 Composition

In the composition calculation, the anisotropy should also be taken into account. For this reason, anisotropic diffusion equations were derived in chapter 4 and implemented and tested in chapter 5. In the implementation, however, a number of terms have been omitted with respect to the derived equations, as was discussed in chapter 4. Inertia, for example, has been neglected in the diffusion equations. In the Navier Stokes equation, which describes the motion of the plasma bulk, inertia is an important term in the expansion region. Neglecting this term on the species level should therefore be carefully evaluated in the future.

It was found that the composition calculation can give non-physical results in the presence of temperature gradients. Even in the absence of chemical source terms, species number densities are not conserved. Especially at the boundaries large deviations are found. This problem was investigated in chapter 8. It was found that the number of grid cells, the temperature gradient and the splitting of the diffusion velocity in a convective and diffusive part are important factors in the problem. It is expected that the formulation of the species balance in terms of number densities is the cause of the problems. Probably, a formulation in terms of mass fractions would be better. This problem in the composition calculation has to be carefully investigated in the future before modeling of Magnum PSI is possible. When comparing Plasimo to, for example, MHD models, the possibility to calculate the chemical composition is Plasimo’s surplus value. It is therefore really important to solve this problem in the future.
9.3 Temperature

The magnetic field causes anisotropy in both the electron and the ion heat conductivity. This anisotropic heat conduction is not implemented in Plasimo at the moment. In the future, this can be done by making use of the heat conduction coefficients derived in chapter 3.

9.4 Outlook

Before modeling of Magnum PSI is possible, some remaining issues have to be addressed. Especially solution of the composition calculation problem is crucial. Once these remaining issues are solved, different numerical studies can be done on Magnum PSI:

- Determining the influence of neutral background gas on the ion beam.

- When a magnetic field is applied, plasma flowing out of the source cannot expand freely into the source chamber because it is confined by the magnetic field. The consequences of this confinement for the Mach number and shockwave structure of the flow can be investigated.

- As mentioned in chapter 1, the beam diameter of Pilot PSI is too small to reach the strongly coupled regime. The required beam diameter for magnum PSI is in the order of 10 cm. One of the options currently under experimental investigation, is the use of multiple discharge channels in the source. However, this has the disadvantage that it is difficult to obtain one, uniform beam. With the help of a numerical model, the uniformity of the beam under different settings can be studied.
Bibliography


Appendix A

Recent modifications of the flow code

One of the requirements for the modeling of Magnum PSI, is the capability of the model to calculate compressible flows and shock waves. As discussed in chapter 6, Plasimo uses the SIMPLE algorithm together with Karki corrections, which should allow for these kind of calculations. However, it was found that when the flow was compressible, large deviations from mass continuity occurred, which often led to divergence of the model. It appeared that the implementation was not correct. Modifications to correct the Karki correction implementation are discussed in section A.1 and A.2. After these modifications, calculation of compressible flows was possible without deviations from mass continuity, but only up to Mach numbers slightly above one. It was found that this was due to an error in the mass density interpolation. This is discussed in section A.3.

A.1 Calculation of the pressure correction

The idea of the SIMPLE algorithm is that mass density, velocities and pressure are calculated in such a way that mass continuity is fulfilled every iteration step. In the past, in Plasimo this was true only for incompressible flows. For compressible flows, large deviations from mass continuity and convergence problems could be observed. It was found that this was due to the fact that the discretization coefficients were not properly calculated when Karki corrections were switched on.

The first step in calculation of the discretization coefficients (equation 6.14) was determination of the Karki correction coefficient $K$ following:
Kp = urfK * div_gamma * m_bulk->dens(cP) / m_bulk->press(cP);
Ku = urfK * div_gamma * m_bulk->dens(cU) / m_bulk->press(cU);
Kl = urfK * m_bulk->dens(cL) / m_bulk->press(cL);

Then, the velocity correction part (the $\rho^*e$ part in equation 6.14) of the pressure correction discretization coefficient was calculated:

$$
\text{cf.aX}(sU) = m_{bulk->dens_cv()}(cu) * \text{sqr}(Au) * m_{i_ap_v_cv}(cu) * \text{div}_urf;
\text{cf.aX}(sL) = m_{bulk->dens_cv()}(cl) * \text{sqr}(Al) * m_{i_ap_v_cv}(cl) * \text{div}_urf;
$$

The discretization coefficients of the upper (U) and lower (L) neighbors of point $P$ are added to form $a_P$:

$$
\text{cf.aP()} += \text{cf.aX}(sL) + \text{cf.aX}(sU);
$$

Subsequently, the mass density correction (Karki) part of the pressure correction discretization coefficient was calculated:

$$
\text{cf.aX}(sU) += Au * Ku * \text{max}(0.0, -V_{cv}(cu));
\text{cf.aX}(sL) += Al * Kl * \text{max}(0.0, V_{cv}(cl));
$$

and the discretization coefficient $a_P$ is corrected for this:

$$
\text{cf.aP()} += Kp * (\text{max}(V_{cv}(cu), 0.0) * Au
+ \text{max}(-V_{cv}(cl), 0.0) * Al);
$$

As can be seen, the velocity correction part of the discretization coefficient is multiplied by div_urf. This extra underrelaxation caused large deviations from continuity during the iteration process and often led to divergence. Therefore, this factor div_urf has been removed to ensure mass continuity.

### A.2 Compressibility factor

As could be seen in the previous section, a $1/\gamma$ (div_gamma) was used in the calculation of the pressure correction discretization coefficients. Calculated in this way, the Karki correction took into account the influence of the pressure on the mass density as an isentropic process. The $\gamma$ was calculated on the nodal points. After the pressure corrections equation is solved, the pressure correction gives the velocity and the mass density correction. In Plasimo, the mass density correction was carried out with $\gamma$ on the nodal boundaries. This discrepancy caused deviations from mass continuity. Since the precise form of $\rho^*_p$ does not influence the outcome, but only the convergence path of a model, the gamma coefficient has been removed. The Karki correction coefficients now look as follows:
A.3 Interpolation of the mass density

For calculation of the discretization coefficients of the pressure correction equation, the mass density must be known on the cell boundaries. Since in Plasimo the mass density is known on the nodal points, interpolation is needed. In Plasimo, there were two options for mass density interpolation: central differencing and hybrid interpolation as function of the Mach number. The hybrid scheme was meant to give a mixture between central differencing and upstream interpolation for Mach numbers below one and fully upstream interpolation for Mach numbers above one. However, due to an implementation error, fully upstream interpolation was done for Mach numbers below one, while for Mach numbers above one the interpolation was neither upstream nor hybrid. The hybrid interpolation is now done as follows: first the density on the nodal boundaries is determined by upstream interpolation (de_upw):

\[ \text{const double de_upw} = V_{cv}(*\text{pit}) > 0.0 ? \text{dens}(*\text{cL}) : \text{dens}(*\text{cH}), \]

then the density on the nodal boundaries is determined by central differencing (de_cdiff):

\[ \text{const double de_cdiff} = \]
\[ \text{this->gridreg().NodalToSide(dens, comp, *\text{pit}).} \]

After that, the ratio \((upw_e)\) between upstream interpolation and central differencing is calculated from the flow velocity:

\[ \text{const double upw_e} = \min(1.0, \text{fabs}(V_{cv}(*\text{pit}))/c) \]
\[ // \text{const double upw_e} = \max(1.0, \text{sqr}(V_{cv}(*\text{pit}))/c)). \]

The first line gives the new calculation of \(upw_e\), the line that is commented out gives the old (incorrect) calculation. Now the mass density at the nodal boundaries is calculated from \(de_{upw}\), \(de_{cdiff}\) and \(upw_e\):

\[ \text{m_bulk->dens_cv}(*\text{pit}) = upw_e * de_{upw} + (1.0 - upw_e) * de_{cdiff}, \]
as can be seen from the code, this results in the upstream density for Mach numbers above one, central differencing when no flow is present and a combination of central differencing and upstream for Mach numbers between zero and one.

Note that in the derivation of the pressure correction [22] it is assumed that the mass density interpolation is purely upwind. This means pure density upwinding in fact has to be used for mass density interpolation at all velocities. This is now correctly implemented in Plasimo.