IMPLEMENTATION INTO DIVIMP OF A DRIFT-KINETIC MODEL DERIVED FROM THE FOKKER-PLANCK EQUATION TO EXAMINE THE PARALLEL-TO-B VELOCITY COMPONENT OF IMPURITY IONS IN DIVERTOR-TOKAMAK PLASMAS

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
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Implementation into DIVIMP of a Drift-Kinetic Model Derived from the Fokker-Planck Equation to Examine the Parallel-to-B Velocity Component of Impurity Ions in Divertor-Tokamak Plasmas

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Abstract

Dirk Reiser's drift-kinetic (DK) model is compared to the existing fluid approximation (FA) model of the DIVIMP (DIVertor IMPurity) algorithm. The DK model provides a more general equation of impurity ion transport by accounting for the decrease in Coulomb collision cross-sections with increasing relative speed of approaching ions. The FA model is shown to be an approximation of the DK model at low relative speeds. Model comparisons are conducted for carbon ions in strong and weak collisional plasmas using 1) linear temperature and velocity gradients and 2) the Scrape-Off-Layer (SOL) options 12 and 13 of DIVIMP. The steep gradients of weak collisionality were discovered to invalidate the DK model. For strong collisionality with impurities initially at rest both models show no divertor leakage, however, when initial impurity velocities are high the FA model overestimates the Coulomb effects of friction and velocity diffusion and again prevents any upstream leakage of impurities.
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Introduction

The inevitable presence of impurities is an issue that must be addressed if net energy gain from a self-sustaining thermo-nuclear fusion reaction is to be attained. Predictive and analytical tools such as computer modeling coupled with the interpretation of experimental data can assist in determining the size and locations of impurity accumulations within the thermo-nuclear reactors. Such information is invaluable in assessing both the beneficial and harmful effects of impurities. Therefore, a brief introduction to the impact of impurities on a fusion reaction is presented to underscore the need for adequate modeling of their motion.

1.1 Basic Principles of Fusion Reactions Involving Plasmas

Two aspects are involved in attaining controlled fusion reactions in a plasma [1]:

1. Heating of the plasma fuel such that a sufficient number of reacting ions have enough kinetic energy to overcome the Coulomb potential barrier thus allowing the nuclei to get close enough so that the strong nuclear force dominates. Fusion then occurs as some of the mass of the reactants is transformed into the kinetic energy of the products, providing a net energy gain.

2. Maintaining a high enough particle density for a long enough time so that the rate of fusion reaction will liberate more energy than it took to create and confine the plasma.

A favoured candidate reaction is [1]

\[ D + T \rightarrow ^{3}\text{He} (3.5 \text{ MeV}) + n (14.1 \text{ MeV}) \]

Impurities present in the reacting plasma hamper both aspects of the fusion process by

1. reducing the average kinetic energy [2] and
2. diluting the particle density of the fuel ions [2].

However, impurities can also be advantageous as will be discussed below.

1.2 Sources of Impurities

Impurities are created in a number of ways [1]:

- Helium “ash” from the thermo-nuclear reaction.
- Evaporation of atoms from solid surfaces.
• Physical sputtering.
• Chemical sputtering.

1.3 Disadvantages of Impurities

Impurities reaching the core can lead to radiative power losses to the extent that if the impurity content is high enough, the amount of power radiated away would be enough to prevent ignition of the fusing hydrogenic plasma. Such power losses include [1]

• Radiative recombination
• Dielectronic radiation
• Line radiation
• Bremstrahlung radiation
• Cyclotron radiation

Impurities with a low Z, such as beryllium, become completely ionized at temperatures of 1keV [2] and no longer produce line radiation whereas high Z elements, such as tungsten, can still retain their lower orbital electrons even in regions of extremely high temperatures such as the core (up to 10keV) [2]. Thus, the existence of high Z impurities in the core is less tolerable.

The presence of impurities in the core also leads to fuel dilution while impurities near the target plates can lead to self-sputtering. The self sputtering yields can often exceed unity [2] when an impurity having a charge state greater than +1 is accelerated by the plasma sheath potential (at the target surface) to energies much higher than the binding energy of the target atoms. Thus a single impurity can release multiple impurities, which in turn can further contaminate the core.

Co-deposition resulting from the use of carbon materials is another concern since the sink-source mechanism of a solid surface in contact with the hydrogenic plasma is effectively removed [2]. Eroded carbon ions chemically bond to the deposited layer of hydrogenic fuel atoms before they can thermally desorb off of the surface as neutrals. Consequently, recycling of these fuel ions back into the plasma no longer occurs.

1.4 Advantages of Impurities

A primary benefit of impurities is volumetric power losses in the edge plasma [2], [3]. High-energy fuel ions entering the 'scrape off layer' (SOL) and heading toward the divertor targets
impact impurities along the way. The loss in kinetic energy of the fuel ions in exciting and ionizing the impurities reduces the amount of power imparted on the relatively small surface area of the target plates (1 m²) [2]. The resultant multi-directional re-release of this energy in the form of photons (via the radiative processes mentioned above) is thus spread over the larger wall area with no risk of physical sputtering. Therefore, the desired outcome is one in which the impacting fuel ions no longer have sufficient energy to incur physical sputtering or excessive heating of the target surface.

1.5 Motivation for Modeling Techniques

Enhancing the beneficial properties and retarding the harmful effects of impurities requires an accurate means of predicting impurity behaviour under a wide range of plasma conditions for various tokamak configurations. Predicting the locations of impurity ion sources for various charge states is dependent upon their trajectories. This also determines if and where the impurities will accumulate in the SOL (such as upstream at the midpoint where they can then cross-field diffuse into the core) or if they will head to the target plates resulting in either self-sputtering or co-deposition. Conditions could also be such that neutral impurities ionized just in front of the target plates would be drawn back to the plates via the weak electric field (penetrating the plasma from the negatively charged wall) or by the frictional and viscous forces from the plasma flow to the targets. In such an instance, the ionization of the impurities cools the plasma thus reducing the amount of heat that each plasma ion deposits on the target plate. At the same time, the ionization location may be close enough to the targets to prevent the forces in the SOL from accelerating the impurity ions to the energies required to incur self-sputtering. To determine under what conditions such impurity behaviour will occur, it is necessary to know the types and magnitudes of the various forces arising in the SOL. Transport codes can then be developed based on these forces to model impurity ion motion. The results of such predictions can then be compared to experimental findings when such findings are available.

1.6 Thesis Project Motivation and Objective

The objective of this thesis is to add to the existing ion transport code of DIVIMP a new set of equations governing impurity ion transport based on the drift-kinetic (DK) model developed by Dirk Reiser. The motivation stems from the fact that the drift and diffusion coefficients currently employed by the fluid approximation (FA) model of DIVIMP (as derived by Spitzer [4]) only represent the frictional and pressure gradient forces whereas the coefficients of the DK model also include forces arising from variations in the temperature and velocity of the background
plasma ions. This all-inclusive aspect of the DK model is more consistent than the FA model where no viscous force exists and the thermal force component is added separately. The thermal force effect in the FA model is averaged over an ensemble of impurity ions and then divided by \( n_s \) to 'approximate' the force on an individual ion [2] and does not account for the ever changing difference in velocity between the impurity ion and the background plasma. The omission of the thermal and viscous forces from the Spitzer coefficients occurs because he assumed a constant temperature with a constant background plasma flow. Therefore, the parallel velocity diffusion of the FA model also neglects the effects stemming from a temperature and velocity gradient. This then marks the difference of the DK model since it assumes a distorted Maxwellian distribution for the background plasma from which thermal and viscous forces arise automatically due to the inhomogeneities in the background temperature and velocity. These forces then manifest themselves in the drift and diffusive coefficients whereas they must be included separately in the Spitzer analysis. In addition, all the forces of the DK model depend on the normalized difference in the drift velocity between the impurity ion and the background plasma. The FA model assumes this relative velocity will always remain small and is therefore a “small-relative-velocity” approximation of the DK model. Within this range of velocity values, friction increases linearly with speed and the rate of velocity diffusion remains constant. At higher velocities, however, all forces based on Coulomb collisions decrease with increasing speed. Only the DK model accounts for this behaviour and thus offers a more consistent and accurate representation of Coulomb forces for all velocity values.

Additionally, in a Monte Carlo simulation, the exact velocity of the individual impurity is determined at each time increment. In the DK model all the forces acting on an impurity include the effect of this velocity value during each incremental step. This is only true for the standard frictional force used in the FA model (see section 1.4). Therefore, the DK model is more in keeping with the tracking of individual ions.

It has also been demonstrated by Reiser [5], [6] that the thermal averaged force the FA model may, due to its very nature, over-estimate its effect on lower charge state ions because they will not have had sufficient time to thermalize with the background to form a Maxwellian velocity distribution. This then effects the ionization source distribution for the higher charge states (i.e. the lower charge states may be pushed too far into a region of the SOL by the temperature gradient force before being ionized to a higher charge state).

The DK model is thus included as an alternate selection to the FA model currently employed
by DIVIMP.

1.7 Overview of the Thesis Report

Chapter 1 briefly introduces the forces of the FA model. Chapter 2 introduces the DK model with its complete derivation given in Appendix A. It also discusses the conditions of applicability of the DK model with regard to the characteristics of the background plasma into which the impurity ion is to be injected. The conditions are derived in Appendix B. Chapter 2 also shows how making a "small-relative-velocity" approximation of the drift-kinetic time derivatives of the moments $<\Delta v_\phi>$ and $<(\Delta v_\phi)^2>$ leads directly to the form of the Spitzer coefficients used in the FA model of chapter 1. Chapter 3 compares the drift forces of the FA and DK models for single ion motion along a field line under the influence of linear temperature and velocity gradients. Chapter 4 compares the added effect of velocity diffusion. Chapter 5 examines the averaged forces, velocities, and densities along the SOL for 1000 carbon ions in situations of strong and weak collisionality using SOL option 12 and 13 to generate the background plasma. CPU times are also compared. Appendix C shows the dependency of the Trubnikov potentials (used to determine the time derivatives of the moments $<\Delta v_\phi>$ and $<(\Delta v_\phi)^2>$) on the variation in velocity of the impurity ion with respect to the background plasma. Appendix D discusses the major features added to the DIVIMP code to activate the DK model. Various plotting routines available to the user to display the averaged forces and velocities within the edge plasma and to compare the force profiles of both models over a range of velocities are also described in Appendix D.
Chapter 1: Introduction to the Fluid Approximation Model of DIVIMP

DIVIMP (DIVerter IMPurity) is a Monte Carlo code developed by Dr. P.C. Stangeby and J.D. Elder that tracks the motion of individual impurity neutrals and ions in a background plasma, the properties of which are specified as input [7]. The relevant plasma quantities include:

- particle charge, $Z_e$
- particle mass, $m_i$
- particle density, $n_i$
- ion and electron temperature, $T_i$ and $T_e$
- ion flow velocity, $v_i$
- electric field, $E$, which penetrates the plasma from the Debye sheath at the targets

1.1 How the Impurity Ions are Followed

Impurity neutrals that are ionized are tracked through successive states of ionization and recombination until they either deposit on a solid surface or reach the maximum dwell time allocated for observing that particle. The ion's new location and velocity are evaluated at each time increment, $\Delta t$, which is also specified in the input.

1.2 Determination of the Forces in the SOL

When impurity neutrals are ionized their motions are governed by their Coulomb interactions with the ions of the background plasma. Analyzing these interactions Spitzer derived a set of coefficients that describe the drift and diffusive evolution of the impurity velocity distribution [4]. These are the time rate of change of the moments $\langle \Delta v_x \rangle$ and $\langle (\Delta v_x)^2 \rangle$, respectively. These coefficients reflect changes in an ion's velocity rather than its spatial location and can be interpreted to represent the frictional (FF) and pressure gradient (FPG) forces experienced by the impurity. A fuller description of the physical interpretation of the drift and diffusive coefficients is given in Appendix A.2. Spitzer assumed a constant background temperature along with a constant background flow velocity. Thus no allowances were made for forces arising from the temperature and velocity gradients. To remedy this a thermal force term was developed by Braginskii [8] following the Coulomb analysis of Spitzer. Unfortunately, the force is averaged over an ensemble of impurity ions and then divided by the impurity density, $n_i$, to approximate the effect on a single impurity ion. This ion temperature gradient force, FIG, is then added separately to FF and FPG. An analogous electron temperature gradient force, FEG, is also included. The derivation of these thermal forces is presented in chapter 6 of Dr. Stangeby's text:
The Plasma Boundary of Fusion Devices [2]. A similar force can also be constructed from the velocity gradient; however, it is omitted since viscous forces are thought to interact only weakly with impurities. In addition to these Coulomb interactions, the effect of the electric field generated by the electrons coating the surface of the target plates is also included. Some of the field manages to penetrate through the Debye shielding at the target surface and enter the plasma. This results in an electric field force, $FE$, drawing the positive ions to the target.

1.3 Equation of Motion Employed by the Fluid Approximation Model

The force, $F_z$, acting on a single impurity ion of mass $m$, with charge $Z_e e$ moving parallel to the magnetic field, $B$, is the culmination of the forces presented above [9]

$$F_z = FF + FPG + FIG + FEG + FE$$

where

$$FF = m \frac{\bar{v}_z - \bar{v}_z}{\tau_s}$$  \quad \text{(Frictional Force)}  \quad (1.2)$$

$$FPG = -\frac{1}{n_z} \nabla || p_z$$  \quad \text{(Impurity Pressure Gradient Force)}  \quad (1.3)$$

$$FIG = \beta_i \nabla || T_i$$  \quad \text{(Background Ion Temperature Gradient Force)}  \quad (1.4)$$

$$FEG = \alpha_e \nabla || T_e$$  \quad \text{(Background Electron Temperature Gradient Force)}  \quad (1.5)$$

$$FE = Z_e e E_d$$  \quad \text{(Electrostatic Force)}  \quad (1.6)$$

Note that $T$ is in eV, $m$ is in kg, $n$ is in m$^{-3}$, and $p_z$ is in N/m$^2$. Also, $\bar{v}_z$ represents the velocity of a single impurity ion of charge $Z$ while $\bar{v}_z$ represents the average of the local velocity distribution of the background plasma ions. Again, these velocities are strictly parallel to the local magnetic field lines. A more extensive treatment concerning the derivation of these terms is provided by Trubnikov [10], Braginskii [8], and Neuhauser [11]. The directions and magnitudes of these forces are presented schematically in [2] and are reproduced in figure 1 with further embellishment. The resulting change in velocity of the impurity ion is then given as

$$\Delta v_{z||} = \frac{d < \Delta v_{z||} >}{dt} \Delta t + r_G \sqrt{\frac{d < (\Delta v_{z||})^2 >}{dt}} \Delta t + \frac{\beta_i}{m_z} \nabla || T_i \Delta t + \frac{\alpha_e}{m_z} \nabla || T_e \Delta t + \frac{e Z_e}{m_z} E_d \Delta t$$

(1.7)
with the Spitzer coefficients representing the terms corresponding to FF and FPG:

$$\text{FF} \to \frac{d < \Delta v_{zll}>}{dt} = \frac{(\bar{v}_{ll} - \bar{v}_{zll})}{\tau_s} \quad \text{and} \quad \text{FPG} \to \sqrt{\frac{d <(\Delta v_{zll})^2>}{dt} \Delta t} \equiv \sqrt{\frac{kT_z}{m_z}} \sqrt{\frac{2\Delta t}{\tau_q}}$$

where

$$\tau_s = \frac{1.47 \times 10^{13} m_z T_i \sqrt{T_i / m_i}}{(1 + m_i / m_z) n_i Z_z^2 Z_i^2 \lambda} \quad \text{(Spitzer stopping time)} \quad (1.9)$$

$$\tau_q = \frac{1.47 \times 10^{13} m_z T_z \sqrt{T_i / m_i}}{n_i Z_z^2 Z_i^2 \lambda} \quad \text{(Spitzer parallel-to-B velocity diffusion time)} \quad (1.10)$$

For (1.9) - (1.11) \( \tau \) is in seconds, \( T \) is in eV, \( m \) is in a.m.u., and \( n \) is in m\(^{-3}\). Note that the meaning of the notation "< >" employed for the moments differs from that of Spitzer:

$$< \Delta v_{zll} >= \frac{\int \Delta v_{zll} f_i(\bar{v}_i') d\bar{v}_i'}{n_i} \quad \text{where Spitzer denotes} \quad < \Delta v_{zll} >= \frac{d}{dt} \int \Delta v_{zll} f_i(\bar{v}_i') d\bar{v}_i'$$

Also, the thermal gradient force coefficients are

$$\alpha_e = 0.71 Z_e^2 \quad \text{(electrons)} \quad (1.11)$$

$$\beta_i = \frac{3(\mu + 5\sqrt{2} Z_i^2 (1.14^{5/2} - 0.35^{3/2}) - 1)}{2.6 - 2\mu + 5.4 \mu^2} \quad \text{(ions)} \quad (1.12)$$

where \( \mu = \frac{m_z}{m_z + m_i} \quad \text{(reduced mass)} \quad (1.13)$$

and the Coulomb logarithm, \( \lambda = 15 \). Additionally, \( r_G \) is a random number of Gaussian distribution with a mean of 0 and a variance of 1.

The final form of the velocity increment in the FA model is then (2) (with \( T \) in eV, \( m \) in kg, and \( n \) in m\(^{-3}\)):

$$\Delta v_{zll} = \frac{(\bar{v}_{i} - \bar{v}_{z})}{\tau_s} \Delta t + r_G \sqrt{\frac{kT_z}{m_z}} \sqrt{\frac{2\Delta t}{\tau_q}} + \frac{\beta_i}{m_z} \nabla q T_i \Delta t + \frac{\alpha_e}{m_z} \nabla q T_e \Delta t + \frac{Z_z e E}{m_z} \Delta t$$

\[ (1.14) \]
For the velocity equation to be completely valid, the edge plasma must be strongly collisional (i.e. the mean free path between collisions is short compared to the system length, $L_e$, and the gradient scale lengths). Strongly collisional plasmas usually refer to plasmas having a high density and low temperature. Under conditions of low or marginal collisionality "kinetic corrections" must be employed [2]. However, using a Monte Carlo approach [7] allows for greater flexibility in that the ion velocity distribution need not be strictly Maxwellian. The actual velocity distribution is what is being modeled. Additionally, Monte Carlo modeling places no restrictions on the mean free path lengths. Therefore, the approach is termed "quasi-kinetic".
Chapter 2: Introduction to Dirk Reiser's Drift-kinetic Formulation

In response to the shortcomings of the temperature gradient expression used in the FA model, Dirk Reiser derived a set of drift-kinetic equations [5]. These equations provide a kinetic description for the transport of impurity ions in a 'fluid-like' background plasma suitable for implementation in a Monte Carlo algorithm. The interaction of the impurity ions with the background plasma is based on the Coulomb collision term of the Fokker-Planck equation. The drift and diffusive coefficients of this term were evaluated in terms of drift-kinetic variables \(v_\parallel, v_\perp, \) and \(R\), where \(v_\parallel\) and \(v_\perp\) are velocity components parallel and perpendicular to the applied magnetic field and \(R\) is the guiding center position of the ion as it gyrates about the magnetic field line). Furthermore, the impurity ions are taken to interact with a distorted Maxwellian distribution for the background plasma rather than a strictly Maxwellian one, as is the case in a fluid approximation. To include the effect of variations in temperature an additional term is added separately to the FA model. In contrast, the DK model provides a more consistent description of the thermal force because it arises automatically in response to the inhomogeneities in the background temperature (i.e. temperature gradients). This suggested improvement over the existing expression for the thermal force as currently employed in the FA model was one of the main motivating factors for incorporating the Reiser formulation. Additionally, one also obtains an expression for the viscous stress expressed in terms of the background velocity gradient, which again is a result of the distorted Maxwellian. Such an expression is not currently accounted for in the FA model. Thus all the forces arising from Coulomb collisions are completely accounted for in the drift and diffusive coefficients. Additionally, all the forces incorporate the impurity velocity with respect to the background flow and thus are more suitable for a Monte Carlo analysis in which the exact velocity of a single impurity ion is computed [2].

2.1 Equation of Motion Employed by the Drift-kinetic Model

The velocity increment of the DK model implemented into DIVIMP is as follows

\[
\Delta v_{\parallel} = K_4 \Delta t + r_G \sqrt{D_{\|}} \Delta t + \frac{\alpha e}{m_e} \nabla \cdot T_e \Delta t + \frac{Z_e e E_z}{m_z} \Delta t
\]

(2.1)

The drift and diffusive coefficients, \(K_4\) and \(D_{\parallel}\), are obtained from the Trubnikov potentials [10] arising in the Coulomb collision operator of the Fokker-Planck equation. Their complete derivation is presented in Appendix A. \(K_4\) and \(D_{\parallel}\) are a summation of three terms

\[
K_4 = \frac{d}{dt} < \Delta v_{\parallel} > = K_4(a_1) + K_4(\nabla \cdot T_e) + K_4(\nabla \cdot v_{\parallel})
\]

(2.2)
\[ \frac{D_{||}}{dt} <(\Delta v_{z||})^2> = D_{||}(n_i) + D_{||}(\nabla_{||} T_i) + D_{||}(\nabla_{||} v_{z||}) \quad (2.3) \]

where the drift components represent accelerations (in m/s\(^2\)) due to the frictional force, FF,

\[ K_{||}(n_i) = \left(1 + \frac{m_i}{m_z}\right) \lambda \frac{Z_i^2 Z_f^2 e^4}{4 \pi \varepsilon_0^2 m_z T_i} \frac{n_i}{\chi} \left(\frac{\Phi(\chi) - \chi \Phi'(\chi)}{2 \chi^2}\right) \quad (2.4) \]

the ion temperature gradient force, FIG,

\[ K_{||}(\nabla_{||} T_i) = \left(1 + \frac{m_i}{m_z}\right) \frac{3 Z_i^2}{2Z_f^2 m_z} \tilde{\eta}_{||}(1 - 2 \chi_{||}^2) \exp(-\chi_{||}^2) \nabla_{||} T_i \quad (2.5) \]

and the viscous force, FIV (ion velocity gradient force)

\[ K_{||}(\nabla_{||} v_{z||}) = \left(1 + \frac{m_i}{m_z}\right) \frac{3 Z_i^2}{2Z_f^2 m_z} \tilde{\eta}_{||} \sqrt{\pi} \frac{m_i T_i}{2 \chi} \chi \left(\frac{4 \chi - 2 + \frac{3}{2}}{\chi^4} \right) \Phi(\chi) - \frac{3}{\chi^4} \Phi(\chi) \right) \nabla_{||} v_{z||} \quad (2.6) \]

The diffusive components (in m\(^2\)/s\(^3\)) represent diffusion of the velocity (parallel-to-B) associated with the impurity pressure gradient force, FPG,

\[ D_{||}(n_i) = \lambda \frac{Z_i^2 Z_f^2 e^4}{4 \pi \varepsilon_0^2 m_z^2} n_i \sqrt{\pi} \frac{m_i T_i}{2 \chi} \chi \left(\frac{2 \chi - 2 + \frac{3}{2}}{\chi^4} \right) \Phi(\chi) - \frac{3}{\chi^4} \Phi(\chi) \right) \quad (2.7) \]

the ion temperature gradient,

\[ D_{||}(\nabla_{||} T_i) = \frac{3 Z_i^2}{2Z_f^2 m_z^2} \tilde{\eta}_{||} \sqrt{\pi} \frac{m_i T_i}{2 \chi} \chi \left(\frac{2 \chi + 2 + \frac{3}{2}}{\chi^4} \right) \Phi(\chi) - \frac{3}{\chi^4} \Phi(\chi) \right) \nabla_{||} T_i \quad (2.8) \]

and the ion velocity gradient

\[ D_{||}(\nabla_{||} v_{z||}) = \sqrt{\pi} \frac{3 Z_i^2 m_i T_i}{2Z_f^2 m_z^2} \tilde{\eta}_{||} \chi^2 \left(\frac{4}{3 \chi^2} - \frac{10}{3 \chi^4} + \frac{6}{\chi^5}\right) \Phi(\chi) + \left(\frac{2}{3 \chi^3} - \frac{6}{\chi^5}\right) \Phi(\chi) \right) \nabla_{||} v_{z||} \quad (2.9) \]

The quantities within each of these expressions are as follows

- \( e \) Coulomb charge = 1.602 \times 10^{-19} C
- \( \varepsilon_0 \) permittivity of free space = 8.854 \times 10^{-12} F/m
- \( \tilde{\eta}_{||} \) numerical ion viscosity coefficient as given by Balescu [12] = 1/(1.2 + 0.8485Z_i^{-1})
- \( \tilde{\eta}_{||} \) numerical thermal ion conductivity coefficient as given by Balescu [12] = 1/0.5657
A Coulomb logarithm \( \lambda \) = 15

\( m_b \) background ion mass (kg)

\( m_i \) mass of the impurity ion (kg)

\( n_i \) background plasma particle density \( (m^{-3}) \)

\( T_i \) background ion temperature (J)

\( \nabla_i T_i \) background ion temperature gradient parallel to the magnetic field \( (J/m) \)

\( \nabla_i v_i \) background plasma velocity gradient parallel to the magnetic field \( (1/s) \)

\( Z_i \) charge state of the background plasma

\( Z_x \) charge state of an impurity ion

\( \Phi(\chi) \) error function (see Appendix A.63)

\( \Phi'(\chi) \) derivative of the error function (see Appendix A.67)

\( \chi_{\|} = \alpha(\vec{v}_{\|i} - \vec{v}_{\|b}) \) \hspace{1cm} \text{(2.10)}; \hspace{1cm} \alpha = \frac{m_i}{\sqrt{2T_i}} \hspace{1cm} \text{(2.11)}

\( \chi_{\perp} \) normalized relative velocity vector of the individual impurity ion with respect to the average value of the local velocity distribution of the background plasma ions moving parallel to \( B \)

\( \chi = |\chi_{\|} + \chi_{\perp}| = |\chi_{\perp}| \) since the perpendicular component, \( \chi_{\perp} \), is taken to be 0

\( \alpha \) normalization factor: inverse of the thermal ion speed, \( v_{th} \), of the background plasma \( (s/m) \)

Note: The drift and diffusive coefficients are expanded as Taylor polynomials for small \( \chi_{\perp} \) to prevent division by zero when \( \chi_{\perp} = 0 \).

2.2 Relationship between the Electron Gradient Force and the Electrostatic Force of the Drift-kinetic and the Fluid Approximation Models

The remaining forces in the FA model, namely FEG (1.5) and FE (1.6), have been simply added to the DK model as they are in the FA model.

According to Reiser [5], the reason for the omission of the electron temperature gradient force from the DK model is that the normalized relative velocity, \( \chi_e \), between the impurity and the background electron flow would be much less than 1. This is because the thermal velocity of an electron \( \sqrt{2T_e/m_e} \) is much larger than the difference between the impurity and the electron
flow velocity, $|\vec{v}_z - \vec{v}_e|$. Therefore, $\chi_e = \sqrt{m_e / 2T_e} |\vec{v}_z - \vec{v}_e| << 1$. As a result, $K_{\text{el}} = 0$. Despite this, the transport equations derived in this manner are valid for the electrons and ions, as long as the impurity velocity is very high, such as for helium with 3.5 MeV, will the Coulomb collisions with electrons be stronger than those with the background ions.

The complete drift-kinetic formulation [5] also takes into account the $E\times B$-drift, $\nabla B$-drift, and the curvature-drift as well as the mirror effect, all of which occur for an ion gyrating about a magnetic field line in the presence of an electric field. In contrast, the FA model only considers the parallel-to-$B$ component of the $E$-field emanating from the target plates. Since only the parallel-to-$B$ motion is being considered, these particular drift forces are simply replaced with the FE term from the FA model.

2.3 Conditions of Validity for the Drift-kinetic Model

The derivation of the DK model assumes small perturbations from a Maxwellian when describing the distribution function of the background plasma. This means that in the time on the order of the collision time, the distribution function will become a Maxwellian. The transport equations that are derived using this assumption require that the background plasma quantities do not change significantly in time (on the order of the time between collisions) or over distances comparable to the mean free path between collisions [8]. Considering the spatial requirement, this means that the gradient scale lengths for the variation in temperature and velocity must be much larger than the mean free path. The mean free path for a given region depends on the local values of $T_i$ and $n_i$. As such, these values can also determine the minimum gradient scale length required in that region to ensure the validity of the DK model. The full derivation of the minimum gradient scale lengths is given in Appendix B. The results are as follows

\begin{align}
L_{T_i} &= \frac{T_i}{|\nabla T_i|} \geq L_{T_i}^\text{min} = 4 \times 10^{54} \frac{\tilde{\kappa}_i T_i^2}{\lambda Z_i^4 n_i} \quad (2.12) \\
L_{v_i} &= \frac{v_{th}}{|2\nabla v_{th}|} \geq L_{v_i}^\text{min} = 2.7 \times 10^{54} \frac{\tilde{n}_i T_i^2}{\lambda Z_i^4 n_i} \quad (2.13)
\end{align}
L is in m, v is in m/s, T is in J, and \( n_i \) is in m\(^{-3}\). \( L_{\perp} \) and \( L_v \) are the temperature and velocity gradient scale lengths, \( L_{\perp}^{\min} \) and \( L_v^{\min} \) are the minimum values, and \( v_{\text{th}} = \sqrt{2T_i/m_i} \). The gradient scale lengths and their minimum values must be calculated for each grid cell occupying the SOL and the private plasma. For those cells that fail to meet the criteria, the user is notified and the values of the gradient scale lengths for those cells are written to the .lim file along with the minimum required values. This allows the user to compare the values and adjust the background quantities for \( T, n_i \), and \( v_i \) accordingly. However, the user also has the option of automatically switching to the FA model when the impurity enters those cells in which the DK model is invalid. The result of switching between the models is presented in section 4.3.3 and 5.6.

### 2.4 Derivation of the Fluid Approximation Model from the Drift-kinetic Model for a Maxwellian Distribution of Plasma Ions

The fluid approximation expressions for friction and parallel velocity diffusion for a Maxwellian distribution of plasma ions can be obtained by approximating the more general expressions of the DK model for small values of \( |\chi| \). The derivation of the time derivatives of the moments \( \langle \Delta v_{z\perp} \rangle \) and \( \langle (\Delta v_z)^2 \rangle \) leading to the dynamical friction and the parallel velocity diffusion is shown in Appendix A.7.1. The final results are

\[
\frac{d}{dt} \langle \Delta v_{z\perp} \rangle = -\left(1 + \frac{m_i}{m_i} \right) \Omega n_i \alpha^2 \frac{\chi_{\parallel}}{\chi} \left( \frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \right) = K_{\parallel}(n_i) \text{ eqn. (2.4)} \tag{2.14}
\]

\[
\frac{d}{dt} \langle (\Delta v_z)^2 \rangle = \Omega n_i \alpha^2 \frac{\chi_{\parallel}}{\chi} \left( \frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \right) = D_{\parallel}(n_i) \text{ eqn. (2.7)} \tag{2.15}
\]

where

\[
\Omega = \frac{Z_i^2 Z_e^2 e^4}{4\pi \varepsilon_0 m_e^2} \lambda \tag{2.16}
\]

Expressions (2.14) and (2.15) are identical to those given by Spitzer [4] and depend greatly on

\[
\frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \tag{10}.
\]

For \( |\chi| < 1 \),

\[
\frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \rightarrow \frac{2\chi}{3\sqrt{\pi}} \tag{2.17}
\]
For $|\gamma| > 1$, \[ \frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \rightarrow \frac{1}{2\chi^2} \quad (2.18) \]

Under conditions of strong collisionality the velocity of the impurity will not differ significantly from that of the background plasma. Therefore, $|\gamma|$ will be small and

\[
\frac{d}{dt} <\Delta v_{\text{all}}^2> = -\left(1 + \frac{m_z}{m_i}\right) \frac{\Omega n_i \alpha^2 Z_i^2 \chi}{\chi} \frac{2\chi}{3\sqrt{\pi}} \left(1 + \frac{m_i}{m_z}\right) \frac{n_i Z_i^2 Z_z^2}{m_z T_i} \sqrt{\frac{m_i}{T_i}} \left(\bar{v}_{\text{all}} - \bar{v}_{\text{all}}\right)
\]

\[= \frac{\bar{v}_{\text{all}} - \bar{v}_{\text{all}}}{\tau_s} \text{ where } \tau_s = \frac{1.47 \times 10^{13} m_z T_i \sqrt{T_i/m_i}}{(1 + m_i/m_z)n_i Z_i^2 Z_z^2 \lambda} \quad (2.19)\]

Similarly,

\[
\frac{d}{dt} <(\Delta v_{\text{all}})^2> = \Omega n_i \alpha \frac{2}{\chi} \frac{2\chi}{3\sqrt{\pi}} = \frac{2k}{1.42 \times 10^{13}} \frac{n_i Z_i^2 Z_z^2 \lambda}{m_z^2} \frac{T_z}{T_i} \sqrt{\frac{m_i}{T_i}}
\]

\[= \frac{2k T_z}{m_z} \frac{1}{\tau_{\parallel}} \text{ where } \tau_{\parallel} = \frac{1.47 \times 10^{13} m_z T_z \sqrt{T_i/m_i}}{n_i Z_i^2 Z_z^2 \lambda} \quad (2.20)\]

$\tau_s$ is the Spitzer stopping time (1.9) and $\tau_{\parallel}$ is the Spitzer parallel velocity diffusion time (1.10). $k$ is the Boltzmann constant, with $T$ in eV, $m$ in a.m.u., and $n$ in m$^{-3}$. Thus, we have obtained the FA model of chapter 1 by taking the small $|\gamma|$ approximation of the DK model. The FA model is then a special case of the more general theory of impurity ion transport valid under conditions of strong collisionality. The DK model takes into account the decrease in friction and velocity diffusion for large values of $|\gamma|$ due to the diminishing cross section of interaction with increasing velocity for particles undergoing Coulomb collisions. The derivation of the Trubnikov potentials in Appendix C, which lead to (2.14) and (2.15), shows explicitly their dependency on the Coulomb cross section's variation with velocity. This behaviour is not represented in the small $|\gamma|$ approximation of the FA model. This is fine for impurity ions entering the plasma with an initial velocity similar to the average velocity of the plasma ions since the strong force of friction under strong collisionality ensures that $|\gamma|$ remains small. However, if an ensemble of impurities described by a Maxwellian distribution enters the plasma then some ions will invariably have a very high velocity. According to the DK model, they will penetrate much further into the plasma.

Tables 1 and 2 show the relationships between the drift forces and the rate of parallel-to-B velocity diffusion of the two models, respectively.
Chapter 3: Comparison of the Drift-kinetic Model to the Fluid Approximation Model in the Absence of Diffusive Forces Using Linear Gradients

In this chapter the forces from the drift components $K_d(n_i)$ (2.4), $K_d(\nabla_i T_i)$ (2.5), and $K_d(\nabla_i v_{id})$ (2.6) of the DK model are compared to their respective counterparts of the FA model. For convenience, let

\[
\begin{align*}
FF_{FA} &= \text{frictional force (1.2)} \\
FI\!G_{FA} &= \text{ion temperature gradient force (1.4)} \\
F_{net_{FA}} &= \text{net force } = FF_{FA} + FI\!G_{FA} \\
v_{z_{FA}} &= \text{impurity ion velocity parallel to } B
\end{align*}
\]

Fluid Approximation model

\[
\begin{align*}
FF_{DK} &= \text{frictional force} \\
FI\!G_{DK} &= \text{ion temperature gradient force} \\
FI\!V_{DK} &= \text{ion velocity gradient force} \\
F_{net_{DK}} &= \text{net force } = FF_{DK} + FI\!G_{DK} + FI\!V_{DK} \\
v_{z_{DK}} &= \text{impurity ion velocity parallel to } B
\end{align*}
\]

Drift-kinetic model

where

\[
\begin{align*}
FF_{DK} &= -\left(1 + \frac{m_i}{m_z}\right) \lambda \frac{Z_e^2 Z_i^2 e^4}{4 \pi \varepsilon_0^2} \frac{n_i}{T_i} \chi \left(\frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \right) \\
FI\!G_{DK} &= \left(1 + \frac{m_i}{m_z}\right) \frac{3Z_e^2}{2Z_i^2} \bar{\nabla}_{||}(1 - 2\chi_{||}^2) \exp(-\chi_{||}^2) \bar{\nabla}_{||} T_i \\
FI\!V_{DK} &= -\left(1 + \frac{m_i}{m_z}\right) \frac{3Z_e^2}{2Z_i^2} \bar{\nabla}_{||} \sqrt{\pi} \frac{m_i T_i}{2} \chi I \left[\left(\frac{4\chi^3}{3} + \frac{2}{\chi} + \frac{3}{\chi^3}\right) \Phi'(\chi) - \frac{3}{\chi^2} \Phi(\chi) \right] \bar{\nabla}_{||} v_{id}
\end{align*}
\]

3.1 Specifications for the Plots of the Drift Forces versus the Relative Difference in Velocities Parallel to B

Because the DK forces are dependent on the normalized difference in velocities, their profiles and those of the FA model are plotted versus $\chi_i$ in figures 3 and 4. D' ions represent the background plasma with C$^{2+}$ acting as the impurity. The background quantities for $n_i$, $T_i$, $\nabla_i T_i$, $v_i$, and $\nabla_i v_{id}$ used to generate the force plots are obtained from the background plasma profiles of figure 2 where
$|\nabla T| = 1.76 \text{ eV/m}$  ($T_{\text{it}} = T_{\text{ef}} = 10 \text{ eV}; T_{\text{in}} = T_{\text{en}} = 100 \text{ eV}$ at the midpoint)

$V_{\text{pl}} = 607 \text{ s}^{-1}$  ($v_{\text{pl}}$ = plasma sound speed $c_{\text{pl}} = \sqrt{k(T_{\text{it}} + T_{\text{ef}})/m_i} = 31000 \text{ m/s}$)

(Note: subscript 'i' and 'u' denote target and upstream values, respectively)

The values from figure 2 are plotted along ring 8, which represents the series of grid cells that approximate the magnetic field line lying closest to the separatrix within the SOL. The figure also shows the region about the midpoint for which $L_{\text{cn}} L_{\text{cm}}$ when $n_i = 10^{18} \text{ m}^{-3}$. As discussed in section 2.3, this represents a region for which the DK model should not be used.

Figures 3 and 4 show the force profiles with $n_i = 10^{18} \text{ m}^{-3}$ (low density) and $n_i = 10^{19} \text{ m}^{-3}$ (high density), respectively, for a) near target regions (low temperature), b) at the midpoint (high temperature) with a positive temperature gradient, and c) at the midpoint with a negative temperature gradient. Thus, the figures range from scenarios of strong ($n_i = 10^{19} \text{ m}^{-3}, T_i = 10 \text{ eV}$) to weak ($n_i = 10^{18} \text{ m}^{-3}, T_i = 100 \text{ eV}$) collisionality. It should be noted that in weak collisionality the temperature gradient is generally much shallower than in this example with higher target temperatures resulting in a steeper velocity gradient. In addition, when $\chi > 0$, $\vec{v}_i < \vec{v}_z$, and when $\chi < 0$, $\vec{v}_i > \vec{v}_z$, and a positive force accelerates particles in the positive direction which is defined as pointing from the outer target to the inner target.

### 3.2 Two Significant Trends of the Drift Forces

From figures 3 and 4, two important properties are immediately apparent:

1. All forces of the DK model approach 0 for large values of $|\chi|$ (>3)
2. $F_{\text{PK}}$ and $F_{\text{IVK}}$ change sign at $|\chi| = 0.707 (=1/\sqrt{2})$ and $|\chi| = 1.2552$, respectively.

### 3.3 Frictional Force

In a plasma for which $v_i = 0$, the force arising from the random, thermal motion of the plasma ions incident on a stationary impurity from the left is equal to the force from those ions incident from the right. The net force is therefore 0. The impurity will obtain a random, thermal velocity as it equilibrates to the background plasma temperature, but it will have no net motion in either direction. However, if the impurity is given an initial net velocity to the right, it will collide with more slower particles in front of it also heading to the right. Since the background velocity is Maxwellian, the number of faster ions colliding with the impurity from behind will decrease. The net force is then directed to the left and the impurity slows to a halt [6]. This then is a dynamical
friction force that acts upon the impurity as it moves through the plasma. Figures 3 and 4 clearly show how \( F_{\text{FA}} \) and \( F_{\text{DK}} \) are identical for values of \( |\chi| \leq 0.1 \). Referring to section 2.4, this is the region in which

\[
\frac{\Phi(\chi) - \chi \Phi'(\chi)}{2\chi^2} \rightarrow \frac{2\chi}{3\sqrt{\pi}} \quad \text{and} \quad F_{\text{DK}} \rightarrow F_{\text{FA}}.
\]

However this small \( |\chi| \) approximation fails for large \( |\chi| \) since it does not take into account the reduction of the force with increasing speed, which is a property of Coulomb collisions. Consequently, for increasing \( |\chi| \), \( |F_{\text{DK}}| \) is maximal when \( |\chi| = 1 \), which in the absence of a background plasma flow translates to \( \nu_z = \nu_b = \sqrt{2T_i/m_i} \). For \( |\chi| > 1 \), \( F_{\text{DK}} \) varies as the impact parameter, \( \rho_z \) (Appendix C.10), obtained from the Rutherford scattering cross section. In such instances, \( F_{\text{DK}} \approx 1/(2\chi^2) \). Figure 5 shows the percentage difference of \( F_{\text{FA}} \) from \( F_{\text{DK}} \). When \( F_{\text{DK}} \) is maximal at \( |\chi| = 1 \), \( F_{\text{FA}} \) differs from \( F_{\text{DK}} \) by 76\%. If 10\% is chosen as the maximum allowable difference, then \( |\chi| \) cannot be larger than 0.4 if \( F_{\text{FA}} \) is to remain valid.

The cross section of momentum transfer between the impurity and the background ions decreases with increasing relative speed because the time for which the particles are close enough to interact (i.e. be repelled by each others respective electrostatic fields) is much shorter and reduces the overall magnitude of their deflection and subsequent change in velocity. Under conditions of strong collisionality where \( n_i \) is high and \( T_i \) is low, the small \( |\chi| \) approximation is sufficient since friction is the dominant force and will accelerate the impurity ion to match the drift velocity of the background plasma, thereby keeping \( |\chi| \) small. Figure 4a shows that at the target, FF forces the value of \( \chi_b \) for which \( F_{\text{net}} = 0 \), to remain close to 0. This is the average value of \( \chi \) that a particle starting from rest will achieve for a set of plasma conditions similar to figure 4a. Even so, should some impurities have a high initial velocity (as would be the case in a Maxwellian distribution of impurity velocities or when impurities are deliberately injected into the SOL for diagnostic purposes) \( F_{\text{FA}} \) will severely overestimate the effect of friction and rule out any possibility of upstream leakage of impurities from the divertor legs. Consequently, the more accurate DK model should be employed whenever possible to account for all velocity values.

### 3.4 Ion Temperature Gradient Force

From (3.2), \( F_{\text{IGDK}} \) is positive and maximal when \( \chi \) is 0, such that a stationary particle dropped
into a temperature gradient would immediately experience a force accelerating it into the
temperature gradient (by 'into' it is meant that the particle moves into a region of higher
temperature), see figure 3a-b. Since the cross section of momentum transfer decreases strongly
with the relative speed of the colliding particles [2] more momentum will be imparted to the
impurity from the slower moving plasma ions coming at it from the cooler side than from the
faster moving ions coming at it from the hotter side.

For values of |κ| < 0.707 = 2^{1/2}, FIGDK accelerates the impurity ion into the positive
temperature gradient but decreases in magnitude as the ion gains speed. This is in sharp contrast
to the constancy of FIGFA. Furthermore, when |κ| > 0.707, FIGDK becomes negative but then
approaches 0 as |κ| → ∞. This suggests that for a large difference in the relative speed, FIGDK
will decelerate the impurity ion heading into the temperature gradient. Reiser has provided a
simple example following the work of Trubnikov [10] to demonstrate how this could be possible.
Let there be a temperature gradient but no background flow so that the speed of the impurity ion
is equal to the relative speed. Let \( v_i \) denote the thermal speed of the background ions incident on
impurity from the right and \( v_t \) denote the thermal speed of the background ions coming from the
left. Let the temperature increase toward the right such that \( v_r > v_l \). The resulting thermal force
directed to the right is then approximately

\[
F_z = \frac{1}{(v_z - v_i)^2} \frac{1}{(v_z - v_r)^2}
\]

(3.4)

Now let \( \epsilon \) be a small increment in speed within the interval \( 0 < \epsilon < \frac{|v_r - v_l|}{2} \).

When \( v_z = v_i + \epsilon \), \( F_z = (v_1 - v_r + \epsilon)^2 - \epsilon^2 > 0 \)

but when \( v_z = v_i + \epsilon \), \( F_z = \epsilon^2 - (v_r - v_1 - \epsilon)^2 < 0 \).

Thus, there is a change of sign in the thermal force for \( v_i < v_z < v_r \). Reiser offers a similar
physical interpretation for this behaviour as was used to describe the frictional force in the
previous section, "A particle moving into the gradient will now collide with more slower particles
in front of it also heading into the gradient. Additionally, if the background velocity is
Maxwellian, then the number of faster ions colliding with the impurity from behind will decrease.
The net force is then directed in the opposite direction to the gradient"[6]. This explains the
decrease in $\text{FIG}_{\text{DK}}$ as the impurity picks up speed and why the force changes sign when $|\vec{v}_z - \vec{v}_i| > 2^{-1/2} v_{th}$ (i.e. $\chi_\parallel > 0.707$).

$\text{FIG}_{\text{DK}}$ also becomes negative when $\chi_\parallel < -0.707$. Assume again that $v_i = 0$. If the impurity in a positive temperature gradient is given an initial velocity directed toward the region of lower temperature, it will, according to figure 3a, experience a retarding thermal force for $-0.707 < \chi_\parallel < 0$. If $|v_i|\parallel$ is initially larger such that $\chi_\parallel < -0.707$, $\text{FIG}_{\text{DK}}$ becomes negative and the impurity will be accelerated into the lower temperature region. Essentially, this means an impurity could impact the target at a velocity much higher than the plasma sound speed. No physical explanation is readily forthcoming for this behaviour and represents a limitation of the DK model. This will not be a problem, however, if $\text{FIG}_{\text{DK}}$ is prevented from becoming the dominant force for large $|\chi_\parallel|$. Figure 3b-c shows the forces based on background conditions for which the DK model is invalid. This corresponds to the region right at the midpoint of figure 2 where $\text{FIG}_{\text{DK}}$ is the dominant force for all values of $\chi_\parallel$. Therefore, $\text{Fnet}_{\text{DK}}$ is negative in the presence of a positive $\vec{V}_\parallel\vec{T}_i$ when $\chi_\parallel < -0.707$, figure 3b, and positive in the presence of a negative $\vec{V}_\parallel\vec{T}_i$ when $\chi_\parallel > 0.707$, figure 3c. It must be remembered that the DK model relies on a background plasma distribution that is close to a Maxwellian. Therefore, the friction, $\text{FF}_{\text{DK}}$, representing collisions between the impurity and an unperturbed Maxwellian distribution of background ions must be the dominant force (except at $\chi_\parallel = 0$ where $\text{FF}_{\text{DK}} \to 0$), figure 3a. $\text{FIG}_{\text{DK}}$ is the “friction” the impurity experiences due solely to the presence of a temperature gradient. The gradient represents a perturbation of the Maxwellian distribution. However, this perturbation must be small and as such $\text{FIG}_{\text{DK}}$ can only manifest itself for values of $|\chi_\parallel|$ close to 0 where $\text{FF}_{\text{DK}} \to 0$. It is through the adherence to the criteria of section 2.3 that the temperature gradient scale length is kept large enough to prevent $\text{FIG}_{\text{DK}}$ from becoming the dominant force and accelerating impurities into cooler regions when $|\chi_\parallel| > 0.707$.

In general, when $\chi_\parallel = 0$, $\text{FIG}_{\text{DK}} \approx 1.5 \times \text{FIG}_{\text{FA}}$. When $|\chi_\parallel| = \frac{1}{2\sqrt{2}}$, $\text{FIG}_{\text{DK}} = \text{FIG}_{\text{FA}}$ and when $|\chi_\parallel| = \frac{1}{\sqrt{2}}$, $\text{FIG}_{\text{DK}} = 0$. The average value of $\text{FIG}_{\text{DK}}$ taken over the interval $0 \leq \chi_\parallel \leq 2^{-1/2}$ for the plasma conditions specified in section 3.1 is
In comparison, the value of $\overline{\text{FIG}_D}$ is $9.25 \times 10^{14} \text{N}$. Thus, $\overline{\text{FIG}_D} = 0.92 \times \text{FIG}_A$. If $\text{FIG}_D$ is taken as the more accurate representation of the thermal force for small $\chi$, then $\text{FIG}_A$ underestimates the thermal force when $|\chi| < \frac{1}{2\sqrt{2}}$ and overestimates the force when $\frac{1}{2\sqrt{2}} < |\chi| \leq \frac{1}{\sqrt{2}}$.

3.5 Ion Velocity Gradient Force

$\text{FIG}_D$ arises from the components of the stress tensor representing that part of the pressure on the impurity due to the deviation of the background plasma velocity distribution from spherical symmetry [8] (see Appendix A.6). The resulting force on the impurity is due to the flux of momentum in the direction of the flow associated with the random thermal motion of the background ions [2]. Examining the profiles of figure 3b and 4b, $\text{FIG}_D$ behaves in a similar fashion to $\text{FF}_D$ by accelerating the impurity to match that of the background flow. This acceleration is in the direction of increasing speed, i.e. toward the targets. However, the strength of the force is lower than that of $\text{FF}_D$ by an order of magnitude for $n_i = 10^{19} \text{m}^{-3}$, figures 4a-c. It is thus the smallest contributing factor under the specified plasma conditions. This changes when $\nabla_\text{i} v_\text{i}$ becomes sufficiently large such as in weak collisionality cases where the target temperatures, $T_\alpha$ and $T_\text{e}$, are high enough leading to a large plasma sound speed at the targets, see section 5.6. In such instances, $\text{FF}_D$ is weak due to the high $T_\alpha$ and $\text{FIG}_D$ becomes the dominant force. This, however, is in violation of the criterion that $L_\alpha \geq L_\text{mi}$ and invalidates the DK model for weak collisionality.

Referring to figure 3b, $|	ext{FIG}_D|$ will reach a maximum value when $\chi_i \sim 0.6$ and then decreases to 0 when $\chi_i = 1.2552$. Again, as with $\text{FIG}_D$ and $\text{FF}_D$, $\text{FIG}_D \to 0$ when $\chi \to \infty$. However, as with $\text{FIG}_D$, the viscous force changes sign for significant differences in the relative speed ($\chi > 1.2552$). A corresponding physical interpretation for this behaviour is currently lacking, but as with $\text{FIG}_D$, this unusual behaviour (namely the acceleration of the impurity against the background flow) will not occur as long as $L_\alpha \geq L_\text{mi}$. This ensures that $\text{FF}_D$ remains the dominant force and acts to decrease $\chi_i$ when $\chi_i$ is large. At present, DIVIMP does not employ a
corresponding viscous (velocity gradient) force, however under the allowed plasma conditions based on the criteria of section 2.3, it can be seen from figures 3a and 2a-c that the contribution of $F_{\text{IV,DK}}$ to $F_{\text{net,DK}}$ is small indeed and can be neglected. Although $F_{\text{FF,DK}}$ and $F_{\text{IV,DK}}$ act to decrease $|\chi_d|$, $F_{\text{IV,DK}}$ is independent of $n_i$ and its overall magnitude increases as $T_i^{1/2}$ (3.3) whereas $F_{\text{FF,DK}}$ decreases as $T_i^{-1}(3.1)$, compare figure 3a-b. Finally, $F_{\text{FF,DK}}$ will always be present even in the absence of an ion velocity gradient.

3.6 Net Force

As mentioned above, $F_{\text{FF,DK}}$ must be the dominant force for large values of $|\chi_d|$ in order for the drift-kinetic model to be valid. This is ensured by the criteria $L_{\text{ni}} \geq L_{\text{ni}}^{\text{min}}$ and $L_{\text{Tn}} \geq L_{\text{Tn}}^{\text{min}}$, which prevent $F_{\text{IG,DK}}$ and $F_{\text{IV,DK}}$ from accelerating the impurity into regions of lower temperatures or against the background flow. At $|\chi_d| < \frac{1}{2\sqrt{2}}$, $|F_{\text{IG,DK}}| > |F_{\text{FF,FA}}|$ since $F_{\text{IG,FA}}$ is taken to be the average value of the thermal force acting on the impurity. Thus $|F_{\text{net,DK}}|$ is always slightly larger than $|F_{\text{net,FA}}|$ for such values of $|\chi_d|$. As $|\chi_d|$ increases, the linear rise of $|F_{\text{FF,FA}}|$ means $|F_{\text{net,FA}}|$ grows unabated while $|F_{\text{net,DK}}|$ approaches 0, due to the more accurate representation of Coulomb collisions. As $n_i$ increases and $T_i$ decreases, both $F_{\text{FF,FA}}$ and $F_{\text{FF,DK}}$ increase, thus diminishing the effect of the temperature and velocity gradient forces. As a result, the slope of $F_{\text{net,DK}}$ matches that of $F_{\text{net,FA}}$ for values of $\chi_d$ about 0, figure 4a. Therefore, the behaviour of the FA and the DK models will be nearly identical under conditions of strong collisionality since friction keeps $|\chi_d|$ small. For large values of $\chi_d$, the drift-kinetic model offers a high-relative-velocity correction to the forces of the fluid approximation with $F_{\text{net,DK}} \to 0$.

3.7 Force Balance Plots along the SOL for an Impurity Ion at Rest

Figure 6 and 7 compare the FA model to the DK model along the length of the SOL when $v_z$ is fixed at 0 for the background plasma conditions specified in section 3.1 with $n_i = 10^{18}$ m$^{-3}$ for figure 6 and $n_i = 10^{19}$ m$^{-3}$ for figure 7. The force profiles show in which direction a stationary impurity ion would be accelerated when launched anywhere along the SOL. When $n_i = 10^{18}$ m$^{-3}$, $F_{\text{net,FA}}$ is directed toward the targets over a distance of 9 metres from either solid surface compared to 11 metres for $F_{\text{net,DK}}$. Thus, there is a slightly higher divertor retention of impurities originating from the targets when employing the DK model with a low density. The opposite occurs when $n_i = 10^{19}$ m$^{-3}$ since $F_{\text{net,FA}}$ is now directed toward the targets over a distance of 32 metres compared to 29 metres for $F_{\text{net,DK}}$. 
At the midpoint, $\chi = v_i = 0$ and increases toward the targets when $v_i$ is held fixed. This results in a decrease in the magnitude of $\mathrm{FIG}_{\mathrm{DK}}$ while $\mathrm{FIG}_{\mathrm{FA}}$ remains constant. $\mathrm{Fnet}_{\mathrm{FA}}$ is directed upstream over a slightly larger distance than $\mathrm{Fnet}_{\mathrm{DK}}$, because the effect of a steep temperature gradient is more pronounced at lower densities. At high densities, where friction dominates, $|\mathrm{FF}_{\mathrm{FA}}|$ becomes larger than $|\mathrm{FF}_{\mathrm{DK}}|$ as one moves away from the midpoint resulting in the slightly higher divertor retention of impurity ions for the FA model.

As $|\chi|$ increases away from the midpoint, it equals 0.707 just in front of the targets resulting in a change in the sign of $\mathrm{FIG}_{\mathrm{DK}}$. This need not be of concern since $\mathrm{FF}_{\mathrm{DK}}$ and hence $\mathrm{Fnet}_{\mathrm{DK}}$ are also directed toward the targets. Therefore, any ion launched in this region with $v_i = 0$ will quickly accelerate to $v_i$ such that $|\chi|$ will again be below 0.707. $\mathrm{FIG}_{\mathrm{DK}}$ will then be directed upstream, counteracting the force of friction as the particle heads to the target.

### 3.8 The Effect of the Temperature Gradient Force on Single Particle Motion

The motion of a single impurity ion under the sole influence of $\mathrm{FIG}_{\mathrm{FA}}$ and $\mathrm{FIG}_{\mathrm{DK}}$ is depicted in figures 7 and 8. Note that this is an unphysical situation in that $\mathrm{FF}$ would always be present. However, the following results are presented simply as a comparison of $\mathrm{FIG}_{\mathrm{FA}}$ to $\mathrm{FIG}_{\mathrm{DK}}$.

**Plot Specifications:**

- Injection of a single $\mathrm{C}^+$ at grid cell 25 ($s = 12.98m$, "deep" injection) along ring 8
- $\mathrm{FIG}$ is the sole acting force with $\nabla T_i = 1.76 \text{ eV/m}$
- $T_\parallel = 10 \text{ eV}, T_\perp = 100 \text{ eV}$ (midpoint)
- No cross-field diffusion (particle motion is thus confined to ring 8)
- No charge exchange or recombination (charge remains fixed)
- Initial impurity ion velocity is 0
- $n_i = 10^{19} \text{ m}^{-3}$ (although $\mathrm{FIG}$ is independent of $n_i$)
- $v_i = \nabla v_i = E = 0$
- $\Delta t = 5 \times 10^{-7} \text{ s}$
- Velover = 1 (tracking of the ion is terminated the moment it changes direction, see Appendix D.2.4)
3.8.1 Impurity Motion under the Sole Influence of the Temperature Gradient Force of the Fluid Approximation Model

Figure 8a shows the thermal force as averaged over each grid cell. Figure 9a shows the resultant impurity velocity also averaged over each grid cell. Although the profiles of $F_{\text{IGFA}}$ and $v_{\text{effA}}$ are only shown for $Z_e = 4$, they are the same for $Z_e = 1, 2, 3, 5,$ and $6$. Only the corresponding magnitudes are different with $F_{\text{IGFA}}$ increasing as $Z_e$ increases.

Under the sole influence of $F_{\text{IGFA}}$, an impurity is continuously accelerated into the gradient, achieving the highest velocity for the highest $Z_e$. It should be made clear from the plot that $F_{\text{IGFA}}$ does not vary with $T_i$ but rather with $\nabla T_i$. Thus for a linear temperature gradient $F_{\text{IGFA}}$ will have the same magnitude at high and low $T_i$ values. Basically then, an impurity launched anywhere within the SOL between the outer target and the midpoint experiences the same magnitude of force and is accelerated by the positive gradient to the midpoint. Crossing the midpoint it will then be decelerated by the negative gradient. When $v_{\text{effA}}$ reaches 0, the particle then changes direction and accelerates back into the gradient. Thus it will exhibit perpetual oscillatory motion about the midpoint, figure 9a.

It should be made clear that in the remaining figures of this chapter, the ion is only tracked from the injection point near the outer target (designated as “Start” in the figure) to the point near the inner target where the impurity reverses its motion (designated by “End”). This was done in preparation for the inclusion of the frictional force in section 3.9. Since a reversal of the particle’s motion changes the sign of the frictional force, the FF profile of the particle’s previous motion could be completely “cancelled”. Only unidirectional motion is therefore considered to prevent any cancellations when examining the forces acting on a single ion.

3.8.2 Impurity Motion under the Sole Influence of the Temperature Gradient Force of the Drift-kinetic Model

Figures 8b-c and 9b-c depict the $F_{\text{IGDK}}$ and resultant velocities for collision options CIOPTR1 and CIOPTR2 as introduced in Appendix D.2.1. Briefly, CIOPTR1 computes the drift-kinetic forces based on the average background values of $n_i, v_i, \nabla v_{\text{bg}}, T_i$, and $\nabla T_i$ assigned to the grid cells that map out the SOL. CIOPTR2 computes the forces at each point within the grid cell that the impurity is located at using more precise values of the background quantities. This is done by linearly interpolating the values between the average values located at the cell centers. This provides a smoother transition of the background values across the cell boundaries. The
motivation for providing these two options is discussed in section 3.8.2.2.

3.8.2.1 Particle Heading up a Positive Temperature Gradient

Starting from the launch point, $F_{DGK}$ is maximal, since $v_t(\text{initial}) = v_i = \chi_t = 0$. $F_{DGK}$ quickly decreases with increasing $v_t$. As this process continues, one would assume that $\chi_t$ will quickly equal 0.707 and that $F_{DGK}$ will become 0. Any further increase in $\chi_t$ would lead to a negative $F_{DGK}$, thereby decreasing $\chi_t$ so that $F_{DGK}$ again equals 0 where it would remain. Thus, at some point between the outer target ($s = 0$ m) and the midpoint ($s < 51$ m), $F_{DGK}$ should vanish and $v_{idK}$ should settle to a terminal velocity. Such is the suggestion as put forth by Reiser [6]. In none of the figures does this occur. Rather $F_{DGK}$ "plateaus" to a nonzero value and the impurity continuously accelerates into the positive temperature gradient. The reason for this is that $\chi_t$ is also proportional to $\alpha = 1/v_{th}$ (2.11) which in turn is proportional to $T_i^{1/2}$. As the impurity moves into regions of higher $T_i$, $\alpha$ decreases tending to decrease $\chi_t$. A balance is quickly achieved between the increase in $v_{idK}$ and the decrease in $\alpha$ such that $\chi_t$ is effectively prevented from achieving 0.707. Instead it will settle on a value just below 0.707, see figure 9b. Consequently, $F_{DGK}$ "asymptotically" approaches, but never attains the value of 0. This behaviour is independent of the magnitude of $v_iT_i$. So long as a gradient exists, $F_{DGK}$ will never vanish. Reiser has acknowledged this upon subsequent correspondence [13].

As a comparison, $F_{D} = 9.25 \times 10^{13}$ N in figure 8a, whereas $F_{DGK}$ starts out at a value of $1.4 \times 10^{17}$ N at the launch point ($s = 12.98$ m) (keeping in mind that this is the value at the instant of release and not the cell averaged value as depicted in the figure) and quickly plateaus to $8.24 \times 10^{19}$ N toward the midpoint, figure 8b. The final velocities at the midpoint are $1.80 \times 10^5$ m/s for the fluid model, figure 9a, and $6.41 \times 10^4$ m/s for CIOPTR1, figure 9b. Thus, in the absence of a retarding frictional force the velocity is almost three times larger for the FA model. Taking $F_{DGK}$ as a more accurate representation of the thermal force, $F_{FA}$ produces a severe overestimation [6].

3.8.2.2 Particle heading down a Negative Temperature Gradient

Upon crossing the midpoint, $T_i$ decreases. The temperature gradient and $F_{DGK}$ become negative. Referring back to figures 3c and 4c, this has the net effect of inverting the $F_{DGK}$ profile about the horizontal $\chi_t$ axis.
A problem now arises because we are faced with two potential outcomes. This is most prominently featured in figures 8b-c and 9b-c and is the basis for having two collision options. Figures 8b and 9b depict the scenario in which for $\chi_\lambda < 0.707$, $\text{FIG}_{DK}$ will decelerate the particle, which decreases $\chi_\lambda$ even further until eventually the ion is brought to a halt ($\chi_\lambda = 0$). Changing direction ($\chi_\lambda < 0$), the ion accelerates back into the gradient and will assume the perpetual oscillatory motion as discussed above for $\text{FIG}_{PA}$. However, if the rate at which the temperature decreases is slightly larger than the rate at which $v_z$ decreases, $\chi_\lambda$ will grow due to the $\alpha$ term. $|\text{FIG}_{DK}|$ will thus decrease in magnitude. Eventually, $\chi_\lambda$ will surpass the value of 0.707 where upon the force changes sign and now accelerates the ion into regions of lower temperature. $\chi_\lambda$ then continues to grow unabated, until the exponential term in (3.2) dominates, where upon $\text{FIG}_{DK}$ abruptly shrinks to zero, as shown in figure 8c, and the ion achieves a terminal velocity directed out of the gradient, as shown in figure 9c.

The net effect of all this is that if an ion finds itself heading down a negative temperature gradient it could either decelerate, stop and accelerate back up the gradient or continue to accelerate down the gradient toward a terminal velocity. This is all dependent on how precisely the background values of $v_n$, $v_1 v_n$, $T_i$ and $V_i T_i$ are evaluated. This was the motivation for creating the two collision options. CIOPTR1 tends to produce the reversal of the particle motion whereas CIOPTR2 tends to produce the attainment of a terminal velocity. This is because for CIOPTR1 $T_i$ remains constant over a grid cell so the sensitive balance involving the rate of decrease between $T_i$ and $v_{zDK}$ is never fully developed as it is when using CIOPTR2. However, it must be remembered that $\text{FIG}_{DK}$ is acting in the absence of $\text{FF}_{DK}$ and that this coupled with the strict adherence to the criteria of section 2.3 will prevent the impurity from attaining a terminal velocity directed toward regions of lower temperature. In fact, the coupling of $\text{FF}_{DK}$ with $\text{FIG}_{DK}$ ensures that CIOPTR1 and CIOPTR2 provide almost identical results as is demonstrated in the following sections and removes the need for the extra degree of precision offered by CIOPTR2.

### 3.9 Particle Motion under the Combined Influence of the Frictional and Temperature Gradient Forces

The development of impurity ion motion in the absence of a background plasma flow is as follows: when a stationary ion is launched into a positive temperature gradient, $\text{FF}_{DK} = 0$ and $\text{FIG}_{DK}$ is positive and maximal. Referring to the physical descriptions of $\text{FF}_{DK}$ and $\text{FIG}_{DK}$ given in sections 3.3 and 3.4, as $v_z$ and $\chi_\lambda$ start to grow, $\text{FF}_{DK}$ increases and $\text{FIG}_{DK}$ decreases. $\text{FIG}_{DK} = 0$
when \( v_2 = 2^{-1/2} v_{\text{th}} \) but \( \text{FF}_{\text{DK}} \) continues to grow reaching a maximum when \( v_2 = v_{\text{th}} \). Thus, a balance is struck between the counteracting forces in the interval \( 0 < \chi_0 < 0.707 \) when \( \text{Fnet}_{\text{DK}} = \text{FF}_{\text{DK}} + \text{FIG}_{\text{DK}} = 0 \). The value of \( \chi_0 \) for which \( \text{Fnet}_{\text{DK}} = 0 \) lies closer to 0.707 for weak collisionality and closer to 0 for strong collisionality. The average value of \( \chi_0 \) for the weak collisionality case shown in figure 11b-c is \(-0.55\) whereas for strong collisionality, \( \chi_0 \) < 0.25, figure 13b-c. The force profiles for weak and strong collisionality are shown in figures 10b-c and 12b-c, respectively. Because collisionality is strong in figure 12b-c, \( \chi_0 \) remains small and \( \text{FIG}_{\text{DK}} \) varies little for a particle heading upstream. Its profile is thus similar in shape to \( \text{FIG}_{\text{FA}} \), figure 12a, but with \( \text{FIG}_{\text{FA}} > \text{FIG}_{\text{FA}} \). The midpoint velocity of the DK model is therefore slightly higher at \(-20000\) m/s compared to \( 16000\) m/s for the FA model, figure 13. In contrast, the weaker presence of \( \text{FF}_{\text{DK}} \) in the weak collisionality scenario of figure 10b-c allows for a larger increase in \( v_2 \). However, this results in a corresponding decrease of \( \text{FIG}_{\text{DK}} \) toward the midpoint. Consequently, the midpoint velocity for the DK model \((-50000\) m/s) is half that of the FA model \((100000\) m/s), figure 11.

The high midpoint velocity represents the limitation of the small \(|\chi_0|\) approximation of the fluid approximation model. In figure 11a, \( \chi_0 \) reaches a maximum value of 1.1 at the midpoint. This happens because \( \text{FF}_{\text{FA}} \) is too weak when \( n_i = 10^{18} \) m\(^{-3}\) to counter the acceleration from \( \text{FIG}_{\text{FA}} \). But at \( \chi_0 \sim 1.1 \), the true value of \( \text{FF}_{\text{FA}} \) must be roughly two times smaller than it actually is according to the percentage difference of figure 5. This means the constant value of \( \text{FIG}_{\text{FA}} \) would accelerate the particle to even higher velocities. Therefore, by not taking into account the Coulomb effect of diminishing forces with increasing velocities, both \( \text{FF}_{\text{FA}} \) and \( \text{FIG}_{\text{FA}} \) greatly overestimate their effect on a particle’s velocity when collisionality is weak. It is therefore advantageous for the fluid approximation model that the temperature gradient is generally shallow for weak collisionality. This is in contrast to the scenario being modeled here. Also, when \( n_i = 10^{19} \) m\(^{-3}\), \( \text{FF}_{\text{FA}} \) is again too strong, keeping \( \chi_0 \) closer to 0 than \( \text{FF}_{\text{DK}} \) such that the midpoint velocity is now lower than that of the DK model.

No variation occurs in \( \text{FIG}_{\text{FA}} \) in either collisionality regimes. As such, since

\[
\chi_0 > \chi_{\text{lo}} = \frac{1}{2\sqrt{2}} (\text{where} \ \chi_{\text{lo}} \ \text{is the value for which} \ \text{FIG}_{\text{DK}} = \text{FIG}_{\text{FA}}), \ \text{FIG}_{\text{FA}} \ \text{overestimates the thermal force for weak collisionality. For strong collisionality,} \ \chi_0 < \chi_{\text{lo}} \ \text{and FIG}_{\text{FA}} \ \text{underestimates the thermal force effect, however the difference between FIG}_{\text{DK}} \ \text{and FIG}_{\text{FA}} \ \text{is much less than for}
weak collisionality.

Also of note is the fact that $\text{FF}_\text{DK}$ prevents $\text{FFG}_\text{DK}$ from accelerating the ion into cooler regions, as was the case in figure 8c. In both collisionality examples given above, the ion’s forward motion past the midpoint into cooler regions is abruptly reversed.

3.10 Particle Motion under the Combined Influence of the Frictional, Temperature Gradient and Velocity Gradient Forces

Inclusion of a background flow adds a velocity gradient force to the DK model. However, under both collisionality regimes, its contribution has little effect. For weak collisionality, FF and FIG remain unaltered near the midpoint for both models, compare figure 14 with figure 10. The presence of $v_i$ means a slightly stronger FF at the injection point which reduces the growth rate of $v_i$ heading upstream. However, $v_i \rightarrow 0$ at the midpoint. That coupled with the a rise $T_i$ leads to a reduction of FF such that the midpoint velocities, figure 15, are only slightly less than that of the previous section where no background flow was present.

In the case of strong collisionality, the initial increase in $\chi_1$ brought on by the presence of $v_i$ means that $\text{FF} > \text{FIG}$, figure 16. Therefore, both models accelerate the impurity ion to the outer target, impacting it with a speed of $\sim30000$ m/s, which is only slightly less than the plasma sound speed value of $31000$ m/s, figure 17. Consequently, the exclusion of a velocity gradient force from the FA model can be justified based on these results.

Comparison of CIOPTR1 with CIOPTR2 shows that there is no appreciable difference between them when $\text{FF}_\text{DK}$ is included with $\text{FIG}_\text{DK}$. Thus the extra degree of precision offered by CIOPTR2 is unnecessary when modeling impurity ion transport with all forces present.
Chapter 4: Impurity Behaviour under the Additional Influence of Velocity Diffusion using Linear Gradients:

In this chapter the rate of increase of velocity diffusion arising from the culmination of the terms (2.7), (2.8), and (2.9) of the velocity diffusion are compared to the small $\lambda\eta$ approximation of the FA model:

$$D_{\eta FA} = \frac{d}{dt} \langle (\Delta v_{z\eta}^2) \rangle = \frac{2kT_z}{m_z} \frac{1}{\tau_\eta}$$ (4.1)

where $\tau_\eta$ is as given in (1.10). Figures 18 and 19 plot these terms and their total, $D_{\eta DK}$, versus $\chi_\eta$. The plot specifications are identical to those of section 3.1.

4.1 Decrease of Velocity Diffusion with Increasing Relative Velocity

All the terms of the DK model approach 0 for large $|\chi_\eta|$ (>3) whereas $D_{\eta FA}$ remains constant. As with the drift forces of the previous chapter, this reduction is due to the diminishment of the Coulomb cross section of momentum transfer for increasing values of the relative velocity. For an impurity with an initial $v_z = 0$, the drift-kinetic forces will keep $\chi_\eta$ below 0.707 as discussed in section 3.9. Its average value lies closer to 0 for strong collisionality (i.e. $\chi_\eta < 0.25$) due to the stronger influence of friction. As such, the differences between the two models for large $|\chi_\eta|$ never appears when all impurities start out with velocities similar to $v_i$ with $L_{\eta i} \geq L_{\eta i}^{\text{min}}$ and $L_{\alpha i} \geq L_{\alpha i}^{\text{min}}$.

4.2 Velocity Diffusion in a Maxwellian Distribution of Plasma Ions

For a stationary impurity ion injected into a plasma, the random thermal motion of the plasma ions displace the impurity's spatial and velocity values. The impurity quickly acquires a random thermal velocity with $T_z$ approaching $T_i$. In a plasma of constant temperature with a constant drift velocity, the velocity distributions of the plasma ions on either side of the impurity will be a Maxwellian having the same $v_{th}$. Although diffusion gives the impurity a random thermal velocity, its net velocity and its average spatial displacement will remain 0 after a time much longer than the mean collision time, $\tau_c$. At any instant though it will have some nonzero value of velocity. When considering an ensemble of impurity particles there will arise a spread in their velocity values and their velocity distribution will adopt the Maxwellian form of the plasma ions into which they have been introduced.
According to the DK model, velocity diffusion in the absence of $\nabla T_i$ and $\nabla v_i$ is strongest when the drift velocity of the impurity equals that of the plasma ($\chi_d = 0$) see figures 18 and 19. In the small $\chi_d$ approximation of section 2.4, $D_i(n_i) \to D_{i,FA}$ as $\chi_d \to 0$. When $\chi_d = 0$, velocity dispersion is identical for both models. As with the drift forces (3.1)-(3.3), velocity diffusion diminishes with increasing $\chi_d$. For $\chi_d > 1$, $D_{i,FA}(n_i)$ varies as $1/(2\chi^3)$. According to Spitzer, more dispersion occurs perpendicular to the ion's motion at higher velocities. In other words $D_{i,FA}(n_i) > D_{i,DK}(n_i)$ for large $\chi_d$. Velocity perpendicular to the magnetic field lines is, however, not being considered, and compared to the FA model where absolutely no decrease in the rate of parallel velocity diffusion occurs, the DK model provides a major improvement. Figure 20 shows the percent difference of $D_{i,FA}$ from $D_{i,DK}(n_i)$. The figure is identical to the percent difference of $F_{FA}$ from $F_{DK}$ in figure 5 with a 10% difference occurring when $\chi_d$ equals 0.4.

4.2.1 Velocity Diffusion in the Presence of a Temperature Gradient

From figures 18 and 19, $D_{i,FA}(\nabla T_i)$ is an odd function about $\chi_d = 0$, due to the occurrence of $\chi_d/\chi$ with inflection points at $\chi_d = -1.6, 0, 1.6$. Assume $v_i = 0$ and that an ensemble of impurity ions is accelerated from rest into regions of higher temperature by FIG. The contribution of $D_{i,FA}(\nabla T_i)$ to $D_{i,DK}(n_i)$ increases the rate of velocity diffusion with increasing $v_i$. Thus, $D_{i,DK}$ actually exceeds $D_{i,FA}$ for small deviations of $\chi_d$ from 0 for ions heading up the gradient. However, as $v_i$ increases further, the rate of diffusion again decreases due to the nature of Coulomb collisions. Thus, the temperature gradient initially increases the rate of diffusion for impurities accelerating into hotter regions. The maximum rate of diffusion occurs when $FF_{DK} = -FIG_{DK}$. Form figure 18a, $D_{i,DK}$ is maximal when $\chi_d > 0.3$. This value corresponds to $F_{net,DK} = 0$ in figure 3a. This mirrors the case involving the strictly Maxwellian distribution of background plasma ions for which $D_{i,DK}$ is maximal when $\chi_d$, $F_{DK}$, and $F_{net,DK}$ are 0. The rate of velocity diffusion is then greatest in the absence of any net force acting on the impurity ions.

Figure 18b-c shows the velocity diffusion profiles when $L_{ni} < L_{ni,\text{ma}}$ corresponding to the region about the midpoint in figure 2 when $n_i = 10^{18}$ m$^{-3}$. $D_{i,DK}$ is negative for various values of $\chi_d$ both greater than and less than 0. As discussed in Appendix B, a negative $D_{i,DK}$ implies that the impurity velocity distribution function, $f_i$, is negative. A negative rate of velocity diffusion has no physical meaning and signifies a set of background plasma conditions for which the drift-kinetic model is invalid. These conditions are the same as for figure 3b-c where $FIG_{DK}$ was also shown to accelerate impurities down the temperature gradient.
4.2.2 Velocity Diffusion in the Presence of a Velocity Gradient

Just as with FIV\textsubscript{DK}, \(D_k(n_i)\) is the smallest contributing component for a given set of allowable background plasma conditions. It is well over an order of magnitude smaller than \(D_k(n_i)\) at low \(T_i\) figures 18a and 19a. It contributes to the diffusion associated with \(D_k(n_i)\) for \(|\chi| < 0.75\) but becomes negative when \(|\chi| > 0.75\). As with \(D_k(n_i)\), \(D_k(n_i)\) can dominate when its associated gradient becomes too steep or when either \(n_i\) and hence \(D_k(n_i)\), decreases or \(T_i\) significantly increases.

4.3 Motion of 1000 C\textsuperscript{+} ions under Weak Collisionality using Linear Gradients

Figure 21 shows the force profiles of both models acting on impurity ions when combined with the effect of velocity diffusion. Figure 22 shows the average impurity ion velocity along the SOL with figure 23 displaying the impurity ion density. 1000 stationary C\textsuperscript{+} ions were injected at 13 metres from the outer target on ring 8, which is the location of the grid cell lying just below the X-point. The background plasma conditions are shown in figure 2 with \(n_i = 10^{18} \text{ m}^{-3}\) and \(L_{Ti} < L_{Ti}^{min}\) about the midpoint.

4.3.1 Impurity Ion Transport as Governed by the Fluid Approximation Model

Figure 21a shows the forces of the FA model. \(\text{FIG}_{FA}\) remains constant all along the SOL while \(|\text{FF}_{FA}|\) decreases to 0 at the midpoint. Thus, \(\text{Fnet}_{FA}\) is positive at the injection point, rising to equal \(\text{FIG}_{FA}\) at the midpoint. As a result, figure 22a shows a steady increase in the impurity velocity heading upstream. The strong \(\text{FIG}_{FA}\) effectively traps the impurities at the midpoint allowing none to reach the inner target. The impurities oscillate about the midpoint so that the net velocity there is 0. This leads to a pronounced density spike at the midpoint, figure 23a. In fact only 24 ions actually reach the outer target impacting it with a velocity of ~25000 m/s—below the target plasma sound speed of 31000 m/s. However, the velocity heading upstream climbs to 60000 m/s heading upstream. This is the same as in section 3.9 where \(\text{FF}_{FA}\) is too weak to prevent \(\text{FIG}_{FA}\) from accelerating the impurities to enormous velocities. Indeed, from figure 22a, \(\chi\) is 0.9 heading into the midpoint for which \(\text{FF}_{FA}\) and \(\text{FIG}_{FA}\) are no longer valid.

4.3.2 Impurity Ion Transport as Governed by the Drift-kinetic Model

Figure 21b shows the forces of the DK model. Because \(D_k(n_i)\) can become negative about the midpoint (see figure 18b-c), it is set to 0 whenever this occurs. As discussed in section 3.4, when \(n_i\) and thus \(D_k(n_i)\) are low, \(\text{FIG}_{DK}\) has the potential to accelerate impurities down the temperature
gradient when impurities with a high velocity (i.e. $\chi_i$ is close to 0.707) cross over the midpoint. Heading downstream, $T_i$ decreases which increases $\chi_i$ to beyond 0.707 resulting in a runaway acceleration to the targets. This is indeed the case since $\mathbb{F}_{\text{DK}}$ is positive at the outer target and negative at the inner target in an attempt to slow down these impurities. The peak in the profile of $|\mathbb{F}_{\text{DK}}|$ at the midpoint is the result of those ions whose $\chi_i$ values remain below 0.707. They are then trapped at the midpoint. As the particle oscillates about the midpoint, it reverses its motion and $\chi_i$ momentarily equals 0. $\mathbb{F}_{\text{DK}}$ is then maximal and directed upstream. It is the velocity diffusion which causes some of the particles to attain a $\chi_i > 0.707$ leading accelerations to the targets. Figure 22b clearly shows the high velocities attained by the impurities with only a marginal decrease very near the targets brought on by $\mathbb{F}_{\text{DK}}$. At the targets $v_e$ is $\sim 50000$ m/s ($= 1.6 \times c_e$). Also, the average value of $\chi_i$ is $\sim 0.7$ near the outer target and well over 0.8 approaching the inner target. 359 ions reached the outer target and 299 ions reached the inner target compared to 24 and 0 for the FA model. Thus, the impurity density at the midpoint is only 64% of that of the FA model. figure 23b. As predicted, the DK model is invalid for this example of weak collisionality.

4.3.3 Combination of the Fluid Approximation and the Drift-kinetic Models

Figure 21c, 21c, and 23c show the force, velocity, and density profiles, respectively, when the FA model replaces the DK model in the region about the midpoint where $L_{ni} < L_{ni}^{\text{min}}$. There is a discontinuity in the force profiles at $s = 24$ metres when the one model replaces the other. This is especially prevalent for $\mathbb{F}_{\text{FI}}$. The force, velocity, and density profiles about the midpoint are identical to 21a, 22a, and 23a, respectively, as would be expected. In addition, there is no ion migration to the inner target. As for the outer divertor leg, $\mathbb{F}_{\text{DK}}$ increases toward the target accelerating 31 impurities to an impact velocity of 23000 m/s. This hybridization offers no significant departure from the results of 4.3.1. Yet because the FA model continues to behave as it did in section 4.3.1 it is not a viable substitute for the DK model about the midpoint. The velocities and thus $\chi_i$ remains high heading to the midpoint. Therefore, both the FA and the DK models are invalid for this example of weak collisionality when combined with a steep temperature gradient.

4.4 Motion of $^{1000}$ C$^{++}$'s under High Collisionality Using Linear Gradients

Figures 24, 25, and 26 show the force, velocity, and density profiles of 1000 C$^{++}$ ions injected at the same location as in the previous case but under conditions of the high collisionality as
depicted in figure 2 with \( n_i = 10^{19} \text{ m}^{-3} \). For these conditions \( L_{ni} > L_{ni}^{\text{min}} \) and \( L_{ni} > L_{ni}^{\text{max}} \) everywhere. Again the effect of velocity diffusion is included.

Figure 24a, b, and c show the results for the FA and the DK options CIOPTR1 and CIOPTR2, respectively. In all three cases the profiles of FF, FIG, and Fnet are similar. \( |\text{FIG}_{\text{DK}}| \) and \( |\text{FF}_{\text{DK}}| \) are slightly larger than \( |\text{FIG}_{\text{FA}}| \) and \( |\text{FF}_{\text{FA}}| \), but the net forces are essentially identical. Indeed, the velocity profiles and average \( \chi_A \) values of figure 25 show little variation between the models. The average impact velocity at the targets is equal to the plasma sound speed, \( c_s \). It is interesting to note that the density profiles of figure 26 increase from the injection point to within 3 metres of the target even though the average velocity increases. One would expect a steady decline in the density as the particles pick up speed. The particles injected into grid cell 25 (centered at \( s = 12.97 \text{ m} \)) will only occupy half the cell as they accelerate downstream. Thus the density calculated over the entire cell area will be less than that of cell 24 (centered at \( s = 6.75 \text{ m} \)). The number of particles that exist per unit time in cell 24 is larger than cell 23 (centered at \( s = 3.15 \text{ m} \)) but the larger cell area means cell 24 will have the smaller density. Nearing the targets, the cell areas continue to decrease but the particles' velocity continues to increase, keeping pace with the background plasma flow. Thus, fewer particles will be counted in each of the successive cells leading to the target. This then generates the declining density profile for impurities within 3 metres of the target surface.

In this example of strong collisionality, the value of \( \chi_A \) never exceeds 0.12 for either model. According to figures 5 and 20, the difference in the magnitudes of \( \text{FF}_{\text{FA}} \) and \( \text{FF}_{\text{DK}} \) and \( \text{D}_{\text{FA}} \) and \( \text{D}_{\text{FA}}(n_i) \) is be less than 2%. Thus, two important points should be noted with regard to strong collisionality for impurity velocities close to the average drift velocity of the background plasma:

1. The validity of the small \( |\chi_A| \) approximation of the FA model is ensured.
2. The DK and the FA models produce identical results.
Chapter 5: Comparison of the Drift-Kinetic and the Fluid Approximation Models under Strong and Weak Collisionality using SOL options 12 and 13

Because strictly linear gradients do not adequately represent plasma conditions along the SOL, SOL option 12 and 13 will be used instead to generate more appropriate background plasma profiles for strong and weak collisionality. This is particularly crucial for weak collisionality since the presence of a steep gradient about the midpoint invalidates the application of either model as was demonstrated in section 4.3.3.

5.1 Methodology Employed by the SOL Options in Establishing the Background Plasma Quantities

Using target values for T_e, T_i, and n_i (as specified in the INPUT .d6i file) for the boundary conditions, the SOL options calculate the values for T_e(s), T_i(s), n_e(s), v_i(s), and E(s) along the B-field line for each flux tube. The quantities are calculated up from each of the targets (s = 0) to the midpoint (s = L_e). If the inner and outer target values differ, then a discontinuity in the distribution will occur at the midpoint. The formulations are as follows (subscript ‘t’ designates target values, subscript ‘u’ designates upstream values, and n_e = n_i = n):

5.1.1 Plasma Temperature [2]

For strong collisionality, T_e(s) = T_i(s) = T(s), so SOL option 12 is used with [2]

\[ T(s) = \left( T_t^{7/2} + \frac{7 \ q_{ll} s}{2 \ \kappa_{oe}} \right)^{2/7} \]  \hspace{1cm} (5.1)

For weak collisionality, T_e(s) ≠ T_i(s) and T_e(s) ≪ T_i(s), so SOL option 13 is used with [7]

\[ T_e(s) = \left[ T_{et}^{7/2} + \frac{7 \ q_{le} s}{2 \ \kappa_{oe}} \right]^{2/7} \]  \hspace{1cm} (5.2)

\[ T_i(s) = \left[ T_{it}^{7/2} + \frac{7 \ q_{li} s}{2 \ \kappa_{oi}} \right]^{2/7} \]  \hspace{1cm} (5.3)

where \( q_{ll} = (2kT_{it} + 5kT_{et}) n_i c_{st} \) (heat flux density in W/m^2) [7]  \hspace{1cm} (5.4)
\[ q_e^i = 5kT_{et} n_i c_{st} \quad \text{(electron heat flux density in W/m}^2\text{)} \quad (5.5) \]

\[ q_i^i = 2kT_{lt} n_i c_{st} \quad \text{(ion heat flux density in W/m}^2\text{)} \quad (5.6) \]

\[ c_{st} = \left[ k(T_{et} + T_{et}) / m_i \right]^{1/2} \quad \text{(plasma sound speed at the targets)} \quad (5.7) \]

\[ \kappa_{oe} = 2000 \text{ is the electron parallel conductivity} \quad (5.8) \]

\[ \kappa_{oi} = 60 \text{ is the ion parallel conductivity} \quad (5.9) \]

Note: the 7/2 value in front of the heat flux density term implies all the heat enters the SOL at the midpoint.

### 5.1.2 Plasma Density

Combining the particle conservation equation [2],

\[ \Gamma(s) = n(s) v_i(s) = n_i c_{st} + \int_0^s S_p(s') ds' \quad (5.10) \]

[where \( S_p(s) = S_o \exp(-s/L_{iz}) \) is the ion source. \( (5.11) \)]

and \( S_o = \frac{-n_i c_{st}}{L_{iz} (1 - \exp(-L_c / L_{iz}))} [7] \quad (5.12) \)

\( L_c = \text{connection length, } L_{iz} = \text{ionization length (is also selected in the INPUT file)} \]

with the momentum equation for strong collisionality [2],

\[ n(s)[2kT(s) + m_i v_i(s)^2] = 4n_i k T_i \quad (5.13) \]

and solving for \( n(s) \) by eliminating \( v_i(s) \), one obtains [2]

\[ n(s)^2 - \frac{4n_i k T_i}{m_i c_s^2} n(s) + \frac{\Gamma^2}{c_s^2} = 0 \quad (5.14) \]

\[ n(s) = \frac{1}{2} \left\{ \frac{-4n_i k T_i}{m_i c_s^2} + \left[ \left( \frac{4n_i k T_i}{m_i c_s^2} \right)^2 - 4\Gamma(s)^2 \right]^{1/2} \right\} \quad (5.15) \]

where \( c_s = [k(T_c(s) + T_i(s))/m_i]^{1/2} [2] \quad (5.16) \)
Similarly for weak collisionality, the momentum equation is [2]

\[
n(s)[k(T_e(s) + T_i(s)) + m_i v_i(s)^2] = 2n_i k(T_e + T_i)
\]

and

\[
n(s) = \frac{1}{2} \left\{ -\frac{2n_i k(T_e + T_i)}{m_i c_s^2} + \left[ \frac{2n_i k(T_e + T_i)}{m_i c_s^2} \right]^2 - 4\Gamma(s)^2 \right\}^{1/2}
\]

### 5.1.3 Plasma Velocity [2]

\[
v_i(s) = \frac{\Gamma(s)}{n(s)}
\]

where \(\Gamma(s)\) can be determined from (5.10) above.

Note: In the current investigation, \(E(s) = 0\) such that \(FE = 0\). Since both models use \(FE\) and \(FEG\), they were excluded from this investigation to allow for better comparisons of the other remaining force terms.

### 5.2 Criteria for Weak and Strong Collisionality

The level of collisionality is determined from the mean free path (mfp) lengths of interacting ions given by [2]

\[
\lambda_{ii} = \frac{10^{16} T_i^2}{n_i}
\]

Weak collisionality can be defined to mean when \(\lambda_{ii}\) is on par with the system length (i.e. \(2L_e = 100\) m for the JET grid used here) or is much larger than the gradient scale lengths. Strong collisionality can be taken to be when \(\lambda_{ii}\) is only a few centimeters when compared to the system length. Additionally, for strong collisionality \(T_i(s) = T_e(s)\) and \(V_i T_i\) is significant (i.e. \(T_e \geq 3T_i\)) whereas for weak collisionality \(T_i(s) \gg T_e(s)\) and \(V_i T_i\) is shallow (i.e. \(T_e \geq 1.5T_i\)) [3], [2].

### 5.2.1 Selection of the Plasma Temperature and Density for Weak Collisionality

Weak collisionality is modeled using SOL option 13 \((T_i \neq T_e)\) with

- \(T_i = 100\) eV
- \(T_e = 10\) eV
- \(n_i = 10^{18}\) m\(^{-3}\)
- \(L_{ix} = 0.05\) m
\[ T_{in} = 115 \text{ eV} \] such that \[ T_i = 1.15T_{in} \] and \( \lambda_i = 100 \text{ m} \), the targets with \( c_s = 72600 \text{ m/s} \). The profiles of the background quantities for weak collisionality are shown in figure 27a.

### 5.2.2 Selection of the Plasma Temperature and Density for Strong Collisionality

Strong collisionality is modeled using SOL option 12 (\( T_i = T_e \)) with

- \( T_e = T_i = 13 \text{ eV} \)
- \( n_i = 10^{19} \text{ m}^{-3} \)
- \( L_{az} = 0.05 \text{ m} \) (normally \( L_{az} \) is determined from \( 0.25/(10^{20}n_i) \) so that \( L_{az(\text{strong})} \neq L_{az(\text{weak})} \) [2])

\[ T_{in} = 39 \text{ eV} \] such that \( T_{in} = 3T_i \) and \( \lambda_i = 17 \text{ cm} \), the targets with \( c_s = 35300 \text{ m/s} \). The profiles of the background quantities for strong collisionality are shown in figure 27b. Values of \( T_{in} = 1 \text{ eV} \) and \( n_i = 10^{20} \text{ m}^{-3} \) were also considered, but unfortunately these values result in supersonic flow near the targets which leads to an imaginary value in the density expression (5.15). To prevent this the square root term in the density is set equal to 0, but this produces a discontinuity in the \( v_i(s) \) and \( n_i(s) \) profiles near the targets. Since this may cause undesired effects with regard to \( \text{FITVDK} \), such a model for strong collisionality was avoided.

### 5.3 Predictions of the Drift-Kinetic Model for Weak and Strong Collisionality

Figures 28 to 29 and 30 to 31 show the drift forces and the diffusive terms versus \( \chi_i \) under conditions of weak and strong collisionality. The background plasma values are taken along ring 14, which represents those magnetic field lines in the SOL situated halfway between the last closed flux surface (LCFS) and the field lines closest to the vessel wall. The figures show the forces at three locations along the ring:

- a) \( s = 0.0661 \text{ m} \) (cell 2 next to the outer target)
- b) \( s = 4.7 \text{ m} \) (cell 25 adjacent to the X-point where ions are to be injected)
- c) \( s = 29 \text{ m} \) (cell 39 just before the midpoint)

### 5.3.1 Drift Forces under Weak Collisionality

In contrast to the linear gradients of chapter 4, \( L_{Ti} > L_{Ti}^{\text{max}} \) everywhere along the SOL for low densities and \( \text{FITVDK} \) does not become the dominant force at the midpoint (compare figure 3b to figure 28c). However, \( L_{ni} < L_{ni}^{\text{max}} \) at the targets and as such \( \text{FITVDK} \) becomes the dominant force there. Essentially, by switching from linear gradients to SOL option 13, the problem in chapter 4 where \( L_{Ti} < L_{Ti}^{\text{max}} \) at the midpoint has been replaced by the situation in which \( L_{ni} < L_{ni}^{\text{max}} \) at the
targets. For any impurity ion launched near the outer target with an initial velocity greater than 10500 m/s (=\sqrt{T_z/m_z} directed toward the target, with \(T_z = 14\) eV), \(\chi_t > 1.2552\) and \(F_{\text{IVDK},t}\), and thus \(F_{\text{netDK},t}\), will accelerate the ion upstream against the background plasma flow, figure 28a. Ions with an initial velocity less than this will be quickly accelerated to the target impacting it at speeds close to \(c_n = 72600\) m/s. Should \(v_z\) be initially less than \(-110000\) m/s (\(T_z = 1500\) eV) \(\chi_t < -1.2552\) and \(F_{\text{IVDK},t}\) will accelerate the impurity downstream to even higher speeds, well over twice that of the background plasma flow. In contrast, the magnitude of \(F_{\text{FDK},t}\) is much less and would not be able to accelerate the ion from rest to \(c_n\) within the distance over which \(L_{ni} < L_{\text{mn}}\). Compared to the maximum value of \(F_{\text{IVDK},t}\) at \(\chi_t \sim 0.6\), \(F_{\text{FDK},t}\) is 15 times smaller in figure 28a. This then demonstrates the limitations of the DK model for weak collisionality when \(L_{ni} < L_{\text{mn}}\).

Upstream, the situation improves as the temperature and velocity gradients decrease. Near the X-point, figure 28b, the slope of \(F_{\text{netDK},t}\) approaches that of \(F_{\text{netFA},t}\) for values of \(\chi_t\) close to 0 and no accelerations down the temperature gradient or against the background flow will occur at any \(v_z\). Near the midpoint, figure 28c, \(|F_{\text{netDK},t}|\) is very close to \(|F_{\text{netFA},t}|\) over the interval \(-0.3 < \chi_t < 0.9\) and both model should behave similarly for impurity ion velocities within this interval.

### 5.3.2 Parallel-to-B Velocity Diffusion under Weak Collisionality

As in the previous section, because \(L_{ni} < L_{\text{ni}}^{\text{mn}}\), no negative values of the rate of parallel velocity diffusion occur at the midpoint as was the case in figure 18b. The magnitude of \(D_{\text{ii}}(\nabla_i T_i)\) remains less than \(D_{\text{ii}}(n_i)\) everywhere along the SOL. This is not the case for \(D_{\text{ii}}(\nabla_i v_i)\) which becomes the dominant term near the targets. Again, this is the consequence of allowing \(L_{ni}\) to be less than \(L_{\text{ni}}^{\text{mn}}\). With the background plasma conditions as given in figure 29a, \(D_{\text{ii}}^{\text{IDK},t}\) becomes negative when \(v_z > -30600\) m/s (\(T_z = 12\) eV) or when \(v_z < -90600\) m/s (\(T_z = 1030\) eV). The maximum value of \(D_{\text{ii}}^{\text{IDK},t}\) is 10 times larger than \(D_{\text{ii}}^{\text{FA},t}\) for \(\chi_t = 0\). Heading upstream, the maximum value of \(D_{\text{ii}}^{\text{IDK},t}\) approaches \(D_{\text{ii}}^{\text{FA},t}\) at the X-point, figure 29b. At the midpoint, figure 29c, the peak value of \(D_{\text{ii}}^{\text{IDK},t}\) is shifted to \(\chi_t = 0.3\) which coincides with the value at which \(F_{\text{netDK},t}\) = 0 in figure 28c. At this value, \(D_{\text{ii}}^{\text{IDK},t}\) is only 5% larger than \(D_{\text{ii}}^{\text{FA},t}\), so again both models will show similar results for small values of \(\chi_t\) in this region.

### 5.3.3 Drift Forces under Strong Collisionality

Under strong collisionality, the values of \(F_{\text{netDK},t}\) and \(F_{\text{netFA},t}\) are almost identical over the interval \(-0.4 < \chi_t < 0.4\) for the entire SOL, figure 30. 0.4 is the value for which \(F_{\text{FA},t}\) differs by 10% from \(F_{\text{FDK},t}\). Because \(\nabla_i T_i\) and \(\nabla_i v_i\) are steepest near the targets, the contributions of \(F_{\text{IGDK},t}\) and \(F_{\text{IVDK},t}\)
to $F_{\text{net}_DK}$ shift the value at which $F_{\text{net}_DK} = 0$ to $\chi_i = 0.1$. This value for $\chi$ decreases heading upstream, falling to 0.03 at the midpoint. Because this is the highest average value that $\chi$ will obtain for an impurity ion released with an initial $v_i \sim v_i$, both the FA and the DK model will produce identical results. If, however, an ion is released with a high velocity such that $|\chi| > 1$, $F_{\text{net}_DK}$ is less than $F_{\text{net}_FA}$ and the particle will traverse a larger distance before it slows down. Thus, for those few particles with an exceptionally high velocity at the X-point, i.e., $v_i = 150000$ m/s ($T_i = 2.8$ keV) such that $\chi_i = 3.5$, more upstream leakage and higher velocity impacts at the targets will occur according to the DK model.

### 5.3.4 Parallel-to-B Velocity Diffusion under Strong Collisionality

The maximum value of $D_{\|_{DK}}$ approaches $D_{\|_{FA}}$ heading upstream, figure 31. Again the diminishing temperature and velocity gradients reduce and almost eliminate the effects of $D_{\perp_1} \nabla T_i$ and $D_{\perp_2} \delta v_{lib}$ heading to the midpoint. If 0.1 is the maximum value attained by $|\chi|$ in the SOL as discussed in section 5.3.3, then the parallel velocity diffusion of both models will be identical. Again, almost no velocity diffusion will take place when $|\chi| = 3.5$ for the drift-kinetic model because almost all diffusion will occur perpendicular to the direction of motion according to Spitzer [4]. This is not reflected by the FA model which uses the small $|\chi|$ value for diffusion to encompass all possible particle velocities.

### 5.4 Force Balance Plots along the SOL for an Impurity Ion at Rest under Weak Collisionality

Figure 32 shows the forces that would act on an impurity released anywhere along ring 14 with an initial velocity of 0. FIG dominates FF for the majority of the SOL and particles released beyond 5 metres (the location nearest the X-point) will leak to the midpoint for both models. $v_i = 0$ at the midpoint and thus $\chi$ will equal 0. Therefore, because $|\text{FIG}_{FA}|$ is the averaged value of the thermal force, $|\text{FIG}_{DK}|$ will be stronger at the midpoint. Only as $|v_i|$ increases significantly at the targets does $|\text{FIG}_{DK}|$ approach and then decrease below $|\text{FIG}_{FA}|$. Within the region where $L_m < L_m^{\text{max}}$, $|\text{IVV}_{DK}|$ surpasses $|\text{FF}_{DK}|$. At the targets $|\text{IVV}_{DK}|$ exceeds $|\text{FF}_{DK}|$ by 1.5 orders of magnitude (not shown in the figure). This significant increase in $|\text{IVV}_{DK}|$ occurs over a distance of less than 5 metres from either target, which is much shorter than the mean free path of 100 metres calculated in section 5.2.1 (this being the defining characteristic of weak collisionality). As a result impact velocities at the targets will be higher for the drift-kinetic model.
5.5 Force Balance Plots along the SOL for an Impurity Ion at Rest under Strong Collisionality

Referring to figure 33, \( F_{\text{netDK}} \sim F_{\text{netFA}} \) over the entire length of ring 14. Taking into account the scaling of FIG, \( F_{\text{net}} \) approaches \( \text{FIG} \) within 20 metres from the midpoint. This is a significant departure from the weakly collisional case in that particles released from the rest near the X-point (\( s = 5 \) metres) will not leak upstream. Under strong collisionality the temperature gradient is steeper approaching the targets than for weak collisionality. Thus there is a more significant rise in the FIG of both models. Again, \( \chi_{\text{H}} \) increases from 0 heading away from the midpoint and becomes proportional to \( T_{\text{i}}^{-1/2} \), becomes larger at the lower target temperatures. \( \chi_{\text{H}} \) exceeds 0.707 within 1 metre of the targets and \( \text{FIG}_{\text{DK}} \) changes sign. This need not be of concern because the velocity of any ion launched there (with \( v_{\text{initial}} = 0 \)) will quickly approach \( v_{\text{t}} \) as it accelerates to the targets. \( \chi_{\text{H}} \) then decreases below 0.707 and \( \text{FIG}_{\text{DK}} \) will again be directed toward regions of higher temperature. As \( T_{\text{i}} \) decreases \( |FF_{\text{DK}}| \) grows and overpowers \( \text{FIG}_{\text{DK}} \) in this region such that \( F_{\text{netDK}} \) remains directed toward the target. Thus, there is strong particle retention in the divertor legs at appreciable distances (\( s \leq 10 \) m) from the targets for both models.

5.6 Motion of 1000 Carbon Ions under Weak Collisionality using SOL option 13

Figures 34, 35, and 36 show the forces, average velocities, and the density, respectively, along ring 14 for 1000 C\(^{+4} \) released from rest near the X-point of the outer divertor leg. Table 3 shows the impurity depositions at the targets. The figures and the table show the results for a) the FA model, b) the DK model, and c) a combination of the two where the FA model replaces the DK model whenever \( L_{\text{m}} < L_{\text{m}}^{\text{max}} \). Figure 34a shows \( F_{\text{netFA}} \) approaching \( \text{FIG}_{\text{FA}} \) over the region extending from the X-point (coinciding with the injection point) to the midpoint. Consequently, significant upstream leakage occurs and figure 36a shows a density peak at the midpoint. Even so, velocity diffusion ensures that the majority of particles reach the targets where the stronger presence of \( FF_{\text{FA}} \) accelerates them to an impact speed of 30000 m/s (\(-40\% \) of \( c_{\text{t}} = 72600 \) m/s), figure 35a. \( F_{\text{netDK}} \) also approaches \( \text{FIG}_{\text{DK}} \) heading to the midpoint but the average value of \( |FIG_{\text{DK}}| \) is 1.3 times higher than \( |FIG_{\text{FA}}| \), figure 34b. This results in impurity retention at the midpoint that is almost two times that of the FA model, figure 36b. Referring to table 3, fewer ions from the DK model deposit on the targets within the maximum ion dwell time of 0.1 seconds. Roughly the same number reach the outer target for both models, but only 28% of the ions migrate all the way to the inner target for the DK model compared to 32% for the FA model. Approaching the targets, \( |FTV_{\text{DK}}| \) grows to the extent that the impact speed is 45000 m/s (\(-60\% \) of
c_m), which is a significant difference compared to the FA model, figure 35b.

The average values of \( \chi_t \) depicted in figure 35 are accurate for ions in near-target regions. However, \( \chi_t \) is a vector and as the ions oscillate about the midpoint \( \chi_t \) averages to zero. Therefore, taking the root-mean-square value of \( \chi_t \), it is found that \( \chi_t^{rms} \) reaches a maximum of 0.22 at the midpoint for the FA model and 0.3 for the DK model. At the targets, figure 35a shows the average \( \chi_t \) value reaching a maximum of 0.35. Therefore, the small \( \chi_t \) approximation of the FA model holds for the entire SOL for this particular example of weak collisionality. By substituting the FA model in place of the DK model when \( L_m < L_m^{rms} \), one obtains the results of figure 34c, 35c, and 36c. This has the same effect as setting \( FV_{DK} = 0 \) in the near-target regions since the force, velocity, and density profiles about the midpoint are identical to those of figures 34b, 35b, and 36b, as would be expected, while the force and velocity profiles near the target reflect those of figure 34a and 35a. Thus, one has the higher particle retention of the DK model at the midpoint coupled with the lower target-impact velocities of the FA model.

Although the combination of the FA model with the DK model offers an immediate solution to the problem of steep gradients, it amounts to nothing more than setting the velocity gradient force to zero and taking the average of the temperature gradient force whenever the corresponding steep gradient is encountered. Additionally, the rates of the parallel velocity diffusion that depend on the gradients are also set to zero. In fact, the FA model is already an approximation of the DK model with \( FIG_{FA} \) being the average value of \( FIG_{DK} \) over the interval \( 0 \leq \chi_t \leq 0.707 \). The combination of the models is then questionable since the effects of the gradients do not change in a continuous fashion when moving from strong to weak collisionality. A more general and consistent transport model is therefore required that encompasses all ranges of collisionality.

### 5.7 Motion of 1000 Carbon Ions under Strong Collisionality using SOL option 12 when the Relative Difference in Velocity is Initially Small

Figures 37, 38, and 39 show the forces, average velocities, and the density of 1000 C^{+4} released from rest near the X-point of the outer divertor leg for strong collisionality. a) shows the results of the FA model while b) and c) depict the DK models CIOPTR1 and CIOPTR2, respectively. All three figures show virtually identical results for the FA and DK models. Indeed, \( \chi_t \) is less than 0.2 with FF being the dominant force. Therefore, both models will give similar results since \( FF_{FA} \) differs from \( FF_{DK} \) by less than 5%. All ions impact the outer target at 30000 m/s, which is
less than \( c_s = 35300 \text{ m/s} \), figure 38. The low value of \( \chi_1 (0.2 < \frac{1}{2\sqrt{2}}) \) means \(|F_{\text{DK}}| \) will be slightly larger than \(|F_{\text{FA}}| \) but then the average value of \(|F_{\text{DK}}| \) is also slightly larger than \(|F_{\text{FA}}| \) such that \( F_{\text{net}} \) is the same for both models, figure 37. Indeed, the density profiles are identical in figure 39. Therefore, the FA model is in good agreement with the DK model for small relative impurity ion velocities under conditions of strong collisionality.

The basic trends in impurity motion for the two collisionality regimes along the SOL for low velocity impurities are summarized schematically in figures 40 and 41.

5.8 Motion of 1000 Carbon Ions under Strong Collisionality using SOL option 12 when the Relative Difference in Velocity is Initially Large

The previous section demonstrated the similarity of the models when the relative impurity ion velocities were small. This is due to the fact that the FA model is a small \( \chi_1 \) approximation of the DK model with respect to FF and \( D_1 \left( n_i \right) \). However, when \( v_2 \gg v_1 \), their respective behaviours are completely different. To show this 1000 C\(^{14} \) ions where released near the X-point as in the previous section. Each particle had an initial speed of 200000 m/s \( (T_z = 5 \text{ keV}) \) with 500 particles directed upstream and 500 directed downstream. This velocity results in a \( \chi_1 \) value of \( +/- 4 \) for which \( F_{\text{DK}} \) is but a fraction of \( F_{\text{FA}} \). Consequently, figure 42a shows none of the ions leaking to the midpoint since \( F_{\text{FA}} \) successfully reverses their upstream motion at \( s = 7 \) metres. In addition, \( F_{\text{FA}} \) effectively decelerates all the ions directed to the target within a metre of the injection point. They are then accelerated over the remaining distance to the target. The average impact speed is thus the same as in the previous section. In contrast, 42b-c shows the ions reaching all the way to the midpoint. Indeed, figure 44 shows a density spike at the midpoint since all ions directed upstream have become effectively trapped there. Heading downstream, \( F_{\text{DK}} \) is entirely positive as it attempts to slow the particles down. Its profile is thus opposite in sign to that of \( F_{\text{FA}} \). Consequently, the average impact velocity in figure 43b-c is \(-150000 \text{ m/s} \) (5 times that of figure 43a). Therefore, the nature of Coulomb collisions can have a profound effect on those few impurity ions that have a high velocity. In an ensemble of impurity ions, some will have a high enough velocity to effectively reach the midpoint and potentially leak into the core even under conditions of strong collisionality. This can be very important in instances where even only few impurity ions reaching the core can be critical. As such the DK model provides a more accurate description of ion transport for all impurity velocities values and therefore should always be used under all collisionality conditions whenever \( L_{\text{T}i} \geq L_{\text{T}i}^{\text{min}} \) and \( L_{\text{ni}} \geq L_{\text{ni}}^{\text{min}} \).
5.9 Density Profiles of the Charge States Attained by 1000 Carbon Ions under Weak Collisionalitiy

Figure 45 shows the density profiles of the various ionization states attained by 1000 C⁺ ions launched from rest near the X-point under the same conditions as in section 6.6. The C⁺ and C² profiles of figure 45a peak at 0.13 and 0.08 particles/m², respectively. This is identical to figure 45c where the FA model replaces the DK model at the injection point. In figure 45b, C⁺ is slightly lower at 0.125 particles/m² while C² is slightly higher at 0.086 particles/m². In addition, the C³ profile is slightly higher at the midpoint. Most notable is higher drift-kinetic C⁺⁺ peak, which is well over twice that of the FA model. The midpoint values of figure 45b are reflected in figure 45c where the drift-kinetic model is used about the midpoint. Essentially, the stronger FIGDK quickly forces more particles upstream, resulting in larger density peaks of the higher charge states at the midpoint. This is in contrast to the results obtained by Reiser [5], [6] but then the plasma conditions he employed included a steeper temperature gradient near the targets. The injection point was also closer to the targets where the increased plasma flow meant the injection was initially greater than $\frac{1}{2\sqrt{2}}$. Because this is the value of $\xi_M$ beyond which FIGFA > FIGDK, his results showed the density peaks of the lower charge states occurring closer to the midpoint for the FA model than for the DK model. Therefore, a general conclusion was drawn that FIGFA always overestimates the effect of the temperature gradient. It must be kept in mind, however, that plasma conditions can be selected to show FIGFA either overestimating or underestimating the thermal force.

Tables 4 and 5 show the number of ionizations and target depositions per charge state for both models. A higher percentage of C⁺⁺ and C⁺⁺ ions deposit out for the FA model demonstrating that the slightly larger FIGDK leads to higher particle retention about the midpoint for the DK model.

5.10 Density Profiles of the Charge States attained by 1000 Carbon Ions under Strong Collisionalitiy

The same investigation as described in the previous section was conducted for strong collisionality, the results of which are shown in figure 46. The profiles of the various charge states are identical for both models. C⁺ quickly ionizes to C² at the injection point resulting in a higher C² peak there. Most ionize to C³ further toward the target with a few reaching charge
state 4. Higher states are not achieved because $T_i < 13$ eV in this region. All the profiles diminish toward the target as the particles gain speed. The difference in the effect of $F_l G_{DK}$ and $F_l G_{FA}$ on the various charge states is not prevalent as it was for weak collisionality because under strong collisionality the friction force is much stronger and renders the difference insignificant.

5.11 Comparison of the CPU Times

Referring to table 6, one sees that for the weak collisionality case of section 5.6, the CPU time for CIOPTR1 and CIOPTR2 are well over twice that of the FA model. This is because more particles were retained about the midpoint for the maximum dwell time of 0.1 s (i.e. 59 as compared to the 18 of the FA model). For the strong collisionality case of section 5.7, both models deposited all the ions on the target in the same amount of time. Still, the CPU times for CIOPTR1 and CIOPTR2 are larger than that of the FA model by 1.5 and 1.7 times, respectively. This is the tradeoff one has when employing the more accurate DK model.
Conclusion

Successful implementation into DIVIMP of Dirk Reiser's drift-kinetic (DK) model of impurity ion transport parallel to the B-field has been achieved. It can be selected as a substitution to the existing fluid approximation (FA) model based on the Spitzer analysis. The user can further select either CIOPTR1, which uses the average value of the background plasma quantities in each of the grid cells that map out the SOL and the private plasma, or CIOPTR2, which calculates the exact values at each point within the cell via linear interpolation of the average values. The DK model is a more accurate model by taking into account the decrease in the Coulomb forces with increasing speed of the impurity ion with respect to the plasma ions. The friction force (FF) and the parallel-to-B velocity diffusion (\(D_B\)) of the FA model are obtained from the DK model by assuming this relative speed, \(|\chi|\), remains well below unity. The FA model is thus invalid for large \(|\chi|\). The thermal force (FIG) of the FA model equals the average value of the drift-kinetic thermal force multiplied by a factor of 0.92. This value is obtained by integrating \(\text{FIG}_{DK}\) over the values of \(\chi\) for which it remains directed towards regions of higher temperature, specifically \(0 \leq \chi \leq 0.707\). Furthermore, the DK model is derived using a fluid description for the background plasma and is thus ideally suited for conditions of strong collisionality in which the plasma quantities do not change significantly in time (on the order of the time between collisions) or over distances comparable to the mean free path between collisions. To ensure that the ion temperature and ion velocity gradients that give rise to the thermal and viscous forces are not too steep, the gradient scale lengths (\(L_{Ti}\) and \(L_{\nu}\)) of each grid cell are compared to a minimum value (\(L_{Ti}^{\text{min}}\) and \(L_{\nu}^{\text{min}}\)) determined from the local plasma quantities within that cell. The user is notified when the gradient scale length of a given cell is less than the minimum value and can opt to substitute the FA model for the DK model in those cells. The FA model, however, also requires strong collisionality if \(|\chi|\) is to remain small. Therefore, under conditions of weak collisionality, both models are essentially invalid.

A linear temperature gradient (1.76 eV/m) and a linear velocity gradient (607 s\(^{-1}\)) were used to compare both models under simulated conditions of strong (\(n_i = 10^{19} \text{m}^{-3}\)) and weak (\(n_i = 10^{18} \text{m}^{-3}\)) collisionality. For strong collisionality, \(|\chi|\) never exceeds 0.12 and both models provide identical results with regard to the values for the forces, velocity, and density of the impurity ions along the selected field line. All C\(^{\text{I+}}\) ions released near the X-point of the outer divertor leg impact the outer target with an average speed just below the plasma sound speed (\(c_s = 35300 \text{ m/s}\)). FF is the dominant force and at the maximum \(\chi\) value, \(\text{FF}_{FA}\) and \(D_{\nu,FA}\) are within 2% of \(\text{FF}_{DK}\) and \(D_{\nu,FA}(n_i)\).
For weak collisionality, FF is small and upstream leakage occurs. Nearing the midpoint \( L_{ni} < L_{ni}^{\text{min}} \) and \( D_{1\text{DK}} \) will become negative while \( \text{FIG}_{\text{DK}} \) accelerates impurities down the temperature gradient impacting the targets at 1.6 times \( c_n \). Substituting in the FA model when \( L_{ni} < L_{ni}^{\text{min}} \) leads to \( \chi_d \) exceeding 0.9 such that midpoint velocities become higher than plasma sound speed at the targets. When \( \chi_d > 0.9 \), FF_{FA} and \( D_{1\text{FA}} \) are 60% larger than FF_{DK} and \( D_{1\text{FA}}(n_i) \). Therefore, both models fail under weak collisionality when employing linear gradients but provide excellent agreement under strong collisionality.

To compare the two models under more accurate plasma conditions, SOL options 12 and 13 were employed to simulate conditions of strong and weak collisionality. For weak collisionality, \( L_{ni} < L_{ni}^{\text{min}} \) near the targets, and the drift-kinetic viscous force (\( \text{FIV}_{\text{DK}} \)) accelerates impurities downstream to speeds (45000 m/s) which are higher than those of the FA model (3000 m/s) for which no corresponding viscous force expression exists. Although the average impact speed at the targets is still less than \( c_n = 72600 \) m/s, the acceleration of ions over such a short distance resulting from Coulomb collisions contradicts the defining feature of weak collisionality, namely that the mean free path (mfp) between collisions is large. For this example, the mean free path length near the targets is 100 metres compared to the 5 metres over which \( L_{ni} < L_{ni}^{\text{min}} \). Substituting in the FA model near the targets means the viscous force is simply eliminated and thus does not provide a theoretically adequate solution. Upstream, \( \text{FIG}_{\text{DK}} \) is slightly stronger than \( \text{FIG}_{\text{FA}} \) and leads to a particle density about the midpoint that is twice that of the FA model. For strong collisionality both models again provided identical results when the impurities had an initial velocity that was close to the average drift velocity of the plasma. Since FF is strong, \( \chi_d \) was kept below 0.2 and all particles impacted the outer target with an average speed that was just below \( c_n = 35300 \) m/s. When impurity ions were injected with an initial velocity that was equivalent to a temperature of 5keV, \( \chi_d \) was 4 and all the ions directed upstream under the influence of the DK model reached the midpoint as opposed to none for the FA model. Additionally, those directed to the target impacted the surface at four times \( c_n \) whereas those of the FA model had an average speed just under \( c_n \). Thus, this example shows FF_{FA} severely overestimating the effect of friction. Consequently, the DK model is superior for modeling Coulomb collisions at high relative velocities.

Allowing C\(^{+1} \) ions to ionize to higher charge states, both models were again compared using SOL option 12 and 13. Under weak collisionality, FF is weak and \( \text{FIG}_{\text{DK}} \) is slightly stronger than \( \text{FIG}_{\text{FA}} \) since \( \chi_d \) is less than the value at which \( \text{FIG}_{\text{DK}} \) equals \( \text{FIG}_{\text{FA}} \). Therefore, more ionization
occurs closer to the midpoint for the DK model. In this example, FTGFA underestimates the thermal force effect. For strong collisionality, the stronger presence of FF overpowers the subtle differences between FTQDK and FTGFA such that the distribution of the various charge states for both models is identical.

The CPU times for both models showed significant differences for SOL options 12 and 13. For weak collisionality, the DK model is over twice as long due to the longer average dwell times of the impurities ions about the midpoint. For strong collisionality, CPU times are much shorter since all ions quickly deposit out onto the targets, yet the DK model is still 1.5 times longer. This is the tradeoff of employing a more accurate model. Therefore, when conditions are such that $L_{ni} \geq L_{n1}^{\text{min}}$ and $L_{ni} \geq L_{n1}^{\text{max}}$, the DK model should always be used. When these conditions fail, reverting to the FA model does not provide a theoretically adequate solution since it amounts to simply neglecting the viscous force and the gradient dependent terms in the velocity diffusion expression in addition to adopting an average value for the thermal force. Even though the viscous force is negligible under strong collisionality, one should not simply assume this to be true for weak collisionality. In addition, FF is small for weak collisionality and hence $\kappa_1$ will not necessarily remain close to 0. This then invalidates the FA model. Therefore, a more general ion transport model is required that encompasses all collisionality regimes for all velocity values.
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    Addison-Wesley Publishing Co. Inc., The Netherlands (1966)
    Inc., San Francisco (1986)
Drift Forces:
\[ m_z \frac{d}{dt} \langle \Delta v_{zll} \rangle = m_z \frac{d}{dt} \left[ \langle \Delta v_{zll} \rangle \left|_{\text{Maxwellian}} + \langle \Delta v_{zll} \rangle \left|_{\nabla_T} + \langle \Delta v_{zll} \rangle \left|_{\nabla_{\nabla z}} \right. \right. \right] \]

<table>
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<th>Components:</th>
<th>Drift-kinetic Model</th>
<th>Fluid Approximation Model</th>
</tr>
</thead>
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<tr>
<td>[ m_z \frac{d}{dt} \langle \Delta v_{zll} \rangle \left</td>
<td>_{\text{Maxwellian}} \right. ]</td>
<td>[ = m_z K_6(n_t) ]</td>
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<tr>
<td>[ m_z \frac{d}{dt} \langle \Delta v_{zll} \rangle \left</td>
<td>_{\nabla_T} \right. ]</td>
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<tr>
<td>[ m_z \frac{d}{dt} \langle \Delta v_{zll} \rangle \left</td>
<td><em>{\nabla</em>{\nabla z}} \right. ]</td>
<td>[ = m_z K_6(\nabla_{\nabla z}) ]</td>
</tr>
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</table>

* Note: \[ m_z K_6(\nabla_T) = \sqrt{2} \left( \int_0^{1/2} m_z K_6(\nabla_T) \, d\chi_{\|} \right) = 0.92 \times \beta_1 \nabla_T \] (see section 3.4)

Table 1 Relationship between the drift forces of the drift-kinetic and the fluid approximation models.
Rate of Parallel-to-B Velocity Diffusion:

\[ \frac{d}{dt} \langle (\Delta v_{\parallel})^2 \rangle = \frac{d}{dt} \left[ \langle (\Delta v_{\parallel})^2 \rangle \right]_{\text{Maxwellian}} + \langle (\Delta v_{\parallel})^2 \rangle_{v_{\parallel}T_i} + \langle (\Delta v_{\parallel})^2 \rangle_{v_{\parallel}v_a} \]

<table>
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<th>Components:</th>
<th>Drift-kinetic Model</th>
<th>Fluid Approximation Model</th>
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</thead>
<tbody>
<tr>
<td>$\frac{d}{dt} \langle (\Delta v_{\parallel})^2 \rangle_{\text{Maxwellian}}$</td>
<td>$D_{\parallel}(n_i)$</td>
<td>$\rightarrow \frac{2kT_z}{m_z} \frac{1}{\tau_{\parallel}}$ when $</td>
</tr>
<tr>
<td>$\frac{d}{dt} \langle (\Delta v_{\parallel})^2 \rangle_{v_{\parallel}T_i}$</td>
<td>$D_{\parallel}(\nabla_i T_i)$</td>
<td>N.A.</td>
</tr>
<tr>
<td>$\frac{d}{dt} \langle (\Delta v_{\parallel})^2 \rangle_{v_{\parallel}v_a}$</td>
<td>$D_{\parallel}(\nabla_i v_{\parallel})$</td>
<td>N.A.</td>
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</table>

**Table 2** Relationship between the parallel-to-B velocity diffusion of the drift-kinetic and fluid approximation models.

<table>
<thead>
<tr>
<th>Number of $^{14}C$ ions reaching the Outer Target</th>
<th>Fluid Approximation Model</th>
<th>Drift-kinetic Model</th>
<th>Drift-kinetic and Fluid Approximation Combination</th>
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<td>628</td>
<td>622</td>
<td>625</td>
<td></td>
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<table>
<thead>
<tr>
<th>Number of $^{14}C$ ions reaching the Inner Target</th>
<th>Fluid Approximation Model</th>
<th>Drift-kinetic Model</th>
<th>Drift-kinetic and Fluid Approximation Combination</th>
</tr>
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<tbody>
<tr>
<td>323</td>
<td>282</td>
<td>286</td>
<td></td>
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</tbody>
</table>

**Table 3** Target depositions occurring from the release of 1000 $^{14}C$ ions into a weakly collisional plasma described by SOL option 13.
**Table 4** Ionizations and depositions of $1000 \text{ C}^+$ ions injected into a weakly collisional plasma when employing the fluid approximation model.

<table>
<thead>
<tr>
<th>Charge state</th>
<th>Fluid Approximation Model</th>
<th>Drift-Kinetic Model (CIOPTR1)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Number entering charge state</td>
<td>Number of depositions</td>
</tr>
<tr>
<td>$\text{C}^{+1}$</td>
<td>1000</td>
<td>6</td>
</tr>
<tr>
<td>$\text{C}^{+2}$</td>
<td>994</td>
<td>355</td>
</tr>
<tr>
<td>$\text{C}^{+3}$</td>
<td>639</td>
<td>291</td>
</tr>
<tr>
<td>$\text{C}^{+4}$</td>
<td>348</td>
<td>328</td>
</tr>
<tr>
<td>$\text{C}^{+5}$</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

**Table 5** Ionizations and depositions of $1000 \text{ C}^+$ ions injected into a weakly collisional plasma when employing the drift-kinetic model (CIOPTR1).

<table>
<thead>
<tr>
<th>Charge state</th>
<th>Weak Collisionality</th>
<th>Strong Collisionality</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CPU</td>
<td>Mean Ion Dwell Time (s)</td>
</tr>
<tr>
<td>Fluid Approximation</td>
<td>144603 s</td>
<td>0.01795</td>
</tr>
<tr>
<td>Drift-Kinetic (CIOPTR1)</td>
<td>306080 s</td>
<td>0.02169</td>
</tr>
<tr>
<td>Drift-Kinetic (CIOPTR2)</td>
<td>326013 s</td>
<td>0.01952</td>
</tr>
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</table>

**Table 6** CPU and mean impurity ion dwell times for the fluid approximation and the drift-kinetic models for the weak and strong collisionality cases of sections 5.6 and 5.7. $1000 \text{ C}^{+4}$ ions were released with $\Delta t = 1 \times 10^{-8}$ s and a maximum dwell time of 0.1 s.
Figure 1 Schematic representation of the magnitudes and directions of the forces in the SOL for regions near the target plate and the midpoint [2]. Profiles along the SOL of the ion and electron temperatures, $T_i$ and $T_e$, the ion density, $n_i$, and the ion velocity, $v_i$, are also shown.
Figure 2 Profiles of the background ion and electron temperatures, $T_i$ and $T_e$, ion velocity, $v_i$, and ion density, $n_i$, used to investigate impurity ion motion when the variation in the plasma quantities is constant. The slopes of the linear ion temperature and ion velocity gradients are 1.76 eV/m and 607 s$^{-1}$, respectively.
Figure 3 Dependency on the relative velocity, $\chi$, of the forces of the drift-kinetic and the fluid approximation models acting on a $C^4$ in a low-density plasma with linear gradients. Forces are shown for plasma conditions near the outer target as well as the midpoint for distances slightly less and slightly greater than the connection length, $L_c$. 
Figure 4  Dependency on the relative velocity, $\chi$, of the forces of the drift-kinetic and the fluid approximation models acting on a $C^+$ in a high-density plasma with linear gradients. Forces are shown for plasma conditions near the outer target as well as the midpoint for distances slightly less and slightly greater than the connection length, $L_c$. 

Outer Target ($s = 0$):  
$ni = 10^{19}$ m$^{-3}$  
$T_i = 10$ eV, $v_i = -31000$ m/s  
Temp. gradient = 1.76 eV/m  
Velocity gradient = 607 1/s

Midpoint ($s < L_c$):  
$ni = 10^{19}$ m$^{-3}$  
$T_i = 100$ eV, $v_i = -300$ m/s  
Temp. gradient = 1.76 eV/m  
Velocity gradient = 607 1/s

Midpoint ($s > L_c$):  
$ni = 10^{19}$ m$^{-3}$  
$T_i = 100$ eV, $v_i = 300$ m/s  
Temp. gradient = -1.76 eV/m  
Velocity gradient = 607 1/s
Figure 5 Percent difference in the frictional force with respect to the normalized relative parallel-to-B velocity, \( \chi_B \), between the fluid approximation model, \( FF_{FA} \), and the drift-kinetic model, \( FF_{DK} \), for impurity ions in a strictly Maxwellian distribution of plasma ions.
Figure 6 Magnitudes and directions of the forces that would act on a stationary C^+4 injected anywhere along the SOL in a low-density plasma with linear temperature (1.76 eV/m) and velocity (607 s^-1) gradients.
Figure 7 Magnitudes and directions of the forces that would act on a stationary C⁺⁺ injected anywhere along the SOL in a high-density plasma with linear temperature (1.76 eV/m) and velocity (607 s⁻¹) gradients.
Figure 8 Profiles of the ion temperature gradient force acting on a single C⁺⁺⁺⁺ heading upstream in the absence of any other forces and with no velocity diffusion. Gradients are linear and the impurity ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 9 Average impurity ion velocity and normalized relative velocity, $\chi_b$, of a single C$^{6+}$ heading upstream under the sole influence of the ion temperature gradient force. Ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 10 Profiles of the frictional, ion temperature gradient, and net forces acting on a single C$_{4+}$ ion heading upstream in the absence of velocity diffusion in a low density plasma ($n_i = 10^{18}$ m$^{-3}$). Ion is tracked from the injection point (Start) to the point where its motion reverses (End).
Figure 11 Average impurity ion velocity and normalized relative velocity, $\chi_2$, of a single C$^{+4}$ heading upstream under the influence of the frictional and ion temperature gradient forces in a low-density plasma ($n_i = 10^{16}$ m$^{-3}$). Ion is tracked from the injection point (Start) to the point where its motion reverses (End).
Figure 12 Profiles of the frictional, ion temperature gradient, and net forces acting on a single C\textsuperscript{+4} heading upstream in the absence of velocity diffusion in a high density plasma (n\textsubscript{i} =10\textsuperscript{19} m\textsuperscript{-3}). Ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 13 Average impurity ion velocity and normalized relative velocity, $\chi_h$, of a single C²⁺ heading upstream under the influence of the frictional and ion temperature gradient forces in a high-density plasma ($n_i = 10^{19} \text{ m}^{-3}$). Ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 14 Profiles of the frictional, ion temperature gradient, ion velocity gradient, and net forces acting on a single $C^{+4}$ heading upstream in the absence of velocity diffusion in a low density plasma ($n_i = 10^{18} \text{ m}^{-3}$). Ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 15 Average impurity ion velocity and normalized relative velocity, $\chi_b$, of a single C$^{+4}$ heading upstream under the influence of the frictional, ion temperature gradient, and ion velocity gradient forces in a low-density plasma ($n_i = 10^{18} \text{ m}^{-3}$). Ion is tracked from the injection point (Start) to the point were its motion reverses (End).
Figure 16 Profiles of the frictional, ion temperature gradient, ion velocity gradient, and net forces acting on a single C\textsuperscript{+4} heading upstream in the absence of velocity diffusion in a high density plasma \((n_i = 10^{19} \text{ m}^{-3})\). Ion is tracked from the injection point to the outer target.
Figure 17 Average impurity ion velocity and normalized relative velocity, $\chi_0$, of a single C$^{+4}$ heading upstream under the influence of the frictional, ion temperature gradient, and ion velocity gradient forces in a high-density plasma ($n_i = 10^{19}$ m$^{-3}$). Ion is tracked from the injection point to the outer target.
Figure 18: Dependency on the relative velocity, $\chi_a$, of the velocity diffusion of the drift-kinetic and the fluid approximation models acting on a C4+ in a low-density plasma with linear gradients. Values are shown for plasma conditions near the outer target as well as the midpoint for distances slightly less and slightly greater than the connection length, $L_c$. 
Figure 19 Dependency on the relative velocity, $\chi_b$, of the velocity diffusion of the drift-kinetic and the fluid approximation models acting on a $C^{+4}$ in a high-density plasma with linear gradients. Values are shown for plasma conditions near the outer target as well as the midpoint for distances slightly less and slightly greater than the connection length, $L_c$. 
Figure 20  Percent difference in the velocity diffusion with respect to the normalized, relative parallel-to-$B$ velocity, $\chi_b$, between the fluid approximation model, $D_{\parallel \text{FA}}$, and the drift-kinetic model, $D_{\parallel}(n)$, for impurity ions in a strictly Maxwellian distribution of plasma ions.
Figure 21 Forces acting on 1000 C⁺ ions released from rest into a low-density plasma ($n_i = 10^{18}$ m⁻³) with linear temperature (1.76 eV/m) and velocity (607 s⁻¹) gradients. Parallel-to-B velocity diffusion is included.
Figure 22 Average velocity and relative velocity, $\chi$, of 1000 C$^{++}$ ions released from rest into a low-density plasma ($n_i = 10^{18}$ m$^{-3}$) with linear temperature (1.76 eV/m) and velocity (607 s$^{-1}$) gradients. Parallel-to-B velocity diffusion is included.
Figure 23 Density profile of 1000 C\textsuperscript{+4} ions released from rest into a low density plasma (n\textsubscript{i} = 10\textsuperscript{18} m\textsuperscript{-3}) with linear temperature (1.76 eV/m) and velocity (607 s\textsuperscript{-1}) gradients. Parallel-to-B velocity diffusion is included.
Figure 24 Forces acting on 1000 C⁺ ions released from rest into a high-density plasma ($n_0 = 10^{19}$ m⁻³) with linear temperature (1.76 eV/m) and velocity (607 s⁻¹) gradients. Parallel-to-B velocity diffusion is included.
Figure 25 Average velocity and relative velocity, $\chi_n$ of 1000 C$^{++}$ ions released from rest into a high-density plasma ($n_i = 10^{19}$ m$^{-3}$) with linear temperature (1.76 eV/m) and velocity ($607$ s$^{-1}$) gradients. Parallel-to-B velocity diffusion is included.
Figure 26 Density profile of 1000 C^{+4} ions released from rest into a high-density plasma ($n_i = 10^{19} \text{ m}^{-3}$) with linear temperature (1.76 eV/m) and velocity (607 $\text{s}^{-1}$) gradients. Parallel-to-B velocity diffusion is included.
Figure 27 Profiles of the background ion and electron temperatures, $T_i$ and $T_e$, ion velocity, $v_i$, ion density, $n_i$, and Mach value used to investigate impurity ion motion under conditions of strong and weak collisionality using SOL option 12 and 13, respectively.
Figure 28 Dependency on the relative velocity, $\chi_k$, of the forces of the drift-kinetic and the fluid approximation models acting on a C++ under conditions of weak collisionality using SOL option 13. Forces are shown for plasma conditions proceeding upstream from the outer target to a distance slightly less than the connection length, L_c, at the midpoint.
Figure 29  Dependency on the relative velocity, $\chi_r$, of the velocity diffusion of the drift-kinetic and the fluid approximation models acting on a C++ under conditions of weak collisionality using SOL option 13. Values are shown for plasma conditions proceeding upstream from the outer target to a distance slightly less than the connection length, $L_c$, at the midpoint.
Figure 30 Dependency on the relative velocity, $\chi_h$, of the forces of the drift-kinetic and the fluid approximation models acting on a C'' under conditions of strong collisionality using SOL option 12. Forces are shown for plasma conditions proceeding upstream from the outer target to a distance slightly less than the connection length, $L_c$, at the midpoint.
Figure 31 Dependency on the relative velocity, $\chi_\text{rel}$, of the velocity diffusion of the drift-kinetic and the fluid approximation models acting on a C$^{14}$ under conditions of strong collisionality using SOL option 12. Values are shown for plasma conditions proceeding upstream from the outer target to a distance slightly less than the connection length, $L_c$, at the midpoint.
Figure 32. Magnitudes and directions of the forces that would act on a stationary C\textsuperscript{++} injected anywhere along the SOL under conditions of weak collisionality using SOL option 13.
Figure 33 Magnitudes and directions of the forces that would act on a stationary $C^{14}$ injected anywhere along the SOL under conditions of strong collisionality using SOL option 12.
Figure 34 Forces and parallel-to-B velocity diffusion acting on 1000 C+4 ions released from rest into a weakly collisional plasma described by SOL option 13.
Figure 35 Average velocity and relative velocity, $\chi_0$, of 1000 C$^{14}$ ions released from rest into a weakly collisional plasma described by SOL option 13.
Figure 36  Density of 1000 C\textsuperscript{14} ions released from rest into a weakly collisional plasma described by SOL option 13.
Figure 37 Forces and parallel-to-B velocity diffusion acting on 1000 C⁺⁺ ions released from rest into a strongly collisional plasma described by SOL option 12.
Figure 38 Average velocity and relative velocity, $\chi_b$, of 1000 C$^{14}$ ions released from rest into a strongly collisional plasma described by SOL option 12.
Figure 39 Density of 1000 C\textsuperscript{4+} ions released from rest into a strongly collisional plasma described by SOL option 12.
Simple Background Plasma Profiles of Density, Temperature, and Velocity:

\[ n_i, T_i, T_e \]

\[ v_i = -c_{st} \quad \longleftrightarrow \quad v_i = 0 \quad \text{Midpoint} \quad v_i = 0 \quad \longrightarrow \quad v_i = c_{st} \]

**Figure 40** Schematic of impurity ion motion along the SOL under strong collisionality:
1) Stationary ions injected in regions where \( FF > FIG \), will accelerate to the nearest target.
2) Ions injected in regions where \( FIG > FF \) will be accelerated to the midpoint.
3) At location A, ions could end up in either region depending on the effect of the random nature of the diffusive force.
4) At location B, ions originating from A are now decelerated by both FIG and FF and thus reverse their direction with no ions transiting to the inner target.
5) Ions will oscillate about the midpoint, location C, leading to a particle build-up.
Figure 41  Schematic of impurity ion motion along the SOL under weak collisionality:
1) Stationary ions injected at location A and D close to where $F_{\text{net}} = 0$ will either accelerate to the target or, depending on the value of the diffusive force, cross into the region where FIG>FF. 2) Ions injected at location B or entering this region from A will be accelerated to the midpoint. 3) Ions from B are now decelerated by FIG and FF and reverse their motion, however, due to the diffusive force some of the ions at location C will continue on to location D and hence deposit on the target. Thus, an ion injected at A could traverse the SOL and be deposited on the inner target.
Figure 42 Forces and parallel-to-B velocity diffusion acting on 1000 $^4$C ions released with an initial velocity of 200000 m/s into a strongly collisional plasma described by SOL option 12. Half the ions are directed upstream with the remainder directed to the outer target.
Figure 43 Average velocity and relative velocity, $\chi_b$, of 1000 C$^+$ ions released with an initial velocity of 200000 m/s into a strongly collisional plasma described by SOL option 12. Half the ions are directed upstream with the remainder directed to the outer target.
Figure 44 Density of 1000 C⁺⁺ ions released with an initial velocity of 200000 m/s into a strongly collisional plasma described by SOL option 12. Half the ions are directed upstream with the remainder directed to the outer target.
Figure 45 Density profiles of the charge states attained by 1000 C$^+$ ions released from rest into a weakly collisional plasma described by SOL option 13.
Figure 46  Density profiles of the charge states attained by 1000 C$^+$ ions released from rest into a strongly collisional plasma described by SOL option 12.
Figure 47 Evolution of a monoenergetic beam of particles injected into a stationary, background plasma having a Maxwellian distribution of velocities [15].
Figure 48 Dependency on the normalized relative velocity, $\chi = |\chi_i|$, of the inverses of the roots $C_1$ and $C_2$. Only $C_1^+$ and $C_2^-$ have two unique values corresponding to positive and negative values of $\chi_i$. 
Figure 49 Change in the relative velocity, $\Delta u_z$, between a test particle and a field particle along the z-axis due to a single Coulomb collision. $u$ and $u'$ are vectors denoting the relative velocity between the particles before and after a collision [10].
Appendix A: Derivation of the Drift-Kinetic Equation Leading to the Coulomb Collision Terms \( K_q \) and \( D_{qq} \)

A.1 Introducing the Drift and Diffusive Coefficients, \( K_q \) and \( D_{qq} \)

As introduced in section 2.1, the velocity increment of the impurity ion involving the Coulomb collision terms \( K_q \) and \( D_{qq} \) as obtained from Dirk Reiser (for applications in a Monte Carlo based algorithm) is of the form

\[
\Delta v_{zq} = K_q \Delta t + \left( D_{qq} \Delta t \right)^{1/2} + \frac{Z_e e E_q}{m_z} \Delta t + \frac{\alpha_e}{m_z} \mathbf{E} \cdot \nabla T_e \Delta t \tag{A.1}
\]

The steps leading to the evaluation of \( K_q \) and \( D_{qq} \) are presented in Reiser's Ph.D. thesis [5], a summary of which is provided in [6]. To obtain a fuller understanding than is provided by the summary, elements of the derivation have been translated from the original work in German. The final forms of \( K_q \) and \( D_{qq} \) have also been reorganized to show more clearly how each of their components depends on the various background plasma quantities.

Reiser starts with the kinetic equation for the impurities in a stationary, background plasma as put forth by Hinton [14]:

\[
\frac{\partial f_z}{\partial t} + \frac{\partial}{\partial x} \left( v_z f_z \right) + \frac{Z_e e}{m_z} \frac{\partial}{\partial v} \left( (\mathbf{E} + v_z \times \mathbf{B}) f_z \right) = \sum_i C_{zi} (f_z, f_i) \tag{5}
\]

\( f_z \) is the single-particle distribution for the impurity ion and \( f_i \) is the particle distribution function of the background plasma (consisting of \( D^+ \) ions). \( E \) and \( B \) are the electric and magnetic fields that permeate the plasma. It is assumed that the conditions and behaviour of the background plasma (i.e. \( n, v_i, \) and \( T_i \)) are known. Only the effects of the background on the impurity will be considered (i.e. the test particle model), neglecting any interactions of the impurity on the background or with other impurities. Such considerations would otherwise lead to non-linear terms arising in \( f_z \) [8]. \( C(f_z, f_i) \) designates the Coulomb interaction of the impurity with the background plasma. Here, the Fokker-Planck form for such an interaction has been used:

\[
C_{zi} (f_z, f_i) = -\sum_p \frac{\partial}{\partial v_p} \left( K_p f_z \right) + \frac{1}{2} \sum_{p,q} \frac{\partial^2}{\partial v_p \partial v_q} \left( D_{pq} f_z \right) \tag{Fokker-Planck collision operator}
\]

\( K_p \) and \( D_{pq} \) are the drift and diffusion coefficients:
Physical Elaboration of the Drift and Diffusive Coefficients

The Coulomb forces in a plasma for both positive and negative charges lead to collective and single-particle interactions. Debye shielding of a given particle effectively screens that particle’s electric field from the rest of the plasma so long as sufficient numbers of particles of opposite charge exist within the Debye sphere surrounding that particle (i.e. a sphere having a radius on the order of the Debye length). At the same time, the long-range nature of the Coulomb force affects most plasma particles equally and simultaneously. This then accounts for the collective behaviour of a plasma. Additionally, there is a noncollective aspect, which occurs when an ion penetrates the Debye sphere of another ion. A binary collision ensues, the effect of which is Debye shielded from the rest of the plasma. Due to the closeness of approach, the impact parameter, ρ, of the one particle with respect to the other will be small resulting in a large scattering angle. Thus, there is the strong Coulomb scattering from a single center (i.e. non-collective behaviour) coupled with the simultaneous weaker scattering from a number of centers (collective behavior) [15].

It is the strong binary collisions that result in the drift and diffusive terms of the Fokker-Planck collision operator. If a monoenergetic beam of particles is injected into a stationary plasma exhibiting a Maxwellian distribution, collisions will cause the mean velocity to decrease to 0 (i.e. drift or frictional effect). Additionally, because the beam particles all started out with the same velocity, collisions will tend to spread out their velocities such that after a given time interval (relaxation time) the beam will have thermalized with the background plasma (i.e. diffusive effect). See figure 47.

A.3 Trubnikov Potential Functions, φ and ψ

Returning to the expressions for the coefficients, (A.4) and (A.5), $m_e$ is the impurity ion mass and $m_i$ is that of the background plasma. Additionally,
\[ \Lambda = \frac{Z_i^2 Z_Z^2 e^4}{4\pi e_0 m_e^2} n_i \quad (m^{-1}s^{-1}) \] (A.6)

where \( \Lambda \) is the Coulomb-logarithm, which is a function of the impact parameter \( p \) for a binary collision [10].

\[ \lambda = \int_0^{\rho_{\text{max}}} \frac{\rho \, dp}{\rho^2 + \rho_{\perp}^2} = \ln \left( \frac{\rho_{\text{max}}}{\rho_{\perp}} \right) \text{ with } \rho(\text{max}) = \lambda D, \text{ the Debye length} \] (A.7)

Numerically, \( \lambda \) is normally taken to be 15, [1].

\( \psi \) and \( \phi \) are the potential functions for the background plasma distribution function, \( f_i(\vec{v}_i) \), as presented by Trubnikov [10],

\[ f_i = \nabla^2 \psi_i \quad \text{and} \quad \phi_i = \nabla^2 \phi_i \] (A.8)

\[ \psi_i(\vec{v}_z) = -\frac{1}{8\pi} \int \frac{f_i(\vec{v}_i) \, d\vec{v}_i}{|\vec{v}_z - \vec{v}_i|} \] (A.9)

\[ \phi_i(\vec{v}_z) = -\frac{1}{4\pi} \int \frac{f_i(\vec{v}_i) \, d\vec{v}_i}{|\vec{v}_z - \vec{v}_i|} \] (A.10)

These differ from the potentials used by Reiser by the omission of \(-1/(4\pi)\) and \(-1/(8\pi)\) for \( \phi_i(\vec{v}_z) \) and \( \psi_i(\vec{v}_z) \) respectively. The derivation of these potentials is provided in Appendix C.

In order to evaluate the potentials and their derivatives, an appropriate form for \( f_i \) must be adopted.

**A.4 Background Plasma Distribution Function**

Generally, a distribution function \( f(\vec{x}, \vec{v}, t) \) when expressed as \( f(\vec{x}, \vec{v}, t) \, d\vec{x}d\vec{v} \) gives the number of particles in a volume element \( d\vec{x}d\vec{v} \) centered at \((x, y, z)\) with velocities between \( v_x + dv_x, v_y + dv_y, \) and \( v_z + dv_z \) at a time \( t \). For a collisional, homogeneous, isotropic plasma in steady state (i.e. unchanged in time such that the distribution function is independent of time), the function for the ions can be expressed as

\[ f_i(\vec{x}, \vec{v_i}) = n_i(\vec{x}) f_i^0(\vec{v}_i) \] (A.11)

where \( n_i(\vec{x}) \) is the particle density and \( f_i^0(\vec{v}_i) \) is the Maxwellian velocity distribution.
\[
f_{i}^{0}(\vec{v}_{i}) = \left( \frac{m_i}{2\pi T_i} \right)^{3/2} \exp \left( -\frac{1}{2} \frac{m_i}{T_i} (\vec{v}_z - \vec{v}_i)^2 \right)
\]

(A.12)

where \(\vec{v}_i\) is the average velocity, or drift velocity, of the background plasma ions. If the plasma is inhomogeneous, then the velocity distribution can be written as a series expansion:

\[
f_{i}(\vec{v}_{i}) = f_{i}^{0}(\vec{v}_{i}) + f_{i}^{1}(\vec{v}_{i}) + f_{i}^{2}(\vec{v}_{i}) + ...
\]

(A.13)

provided that the mean free path between collisions is still much smaller than the gradient scale length for changes in \(\rho_i, \nu_i, T_i\). In other words, the plasma is still in 'local' equilibrium (since it is the collisions which bring the system into such a state) and the first-order perturbative term, \(f_{i}^{1}(\vec{v}_{i})\), will be a function of \(\nabla v_i\) and \(\nabla T_i\), whose values are small [8]. Steep gradients therefore invalidate this methodology. Considering a first-order perturbation, the series expansion reduces to

\[
f_{i}(\vec{v}_{i}) = f_{i}^{0}(\vec{v}_{i}) (1 + \eta(\vec{v}_{i}))
\]

(A.14)

where \(\eta(\vec{v}_{i})\) is the deviation of the local distribution function \(f_{i}(\vec{v}_{i})\) from its local equilibrium state \(f_{i}^{0}(\vec{v}_{i})\).

For convenience let \(\vec{y} = \alpha(\vec{v}_z - \vec{v}_i)\) \quad (Note: \(\chi = |\vec{y}|\))

(A.15)

with \(\alpha = \sqrt{\frac{m_i}{2T_i}}\)

(A.16)

such that \(f_{i}^{0}(\vec{v}_{i}) = \left( \frac{m_i}{2\pi T_i} \right)^{3/2} \exp \left( -\frac{\vec{y}^2}{2} \right)\)

(A.17)

\(\vec{v}_z\) represents the velocity of a single impurity ion of charge \(Z\) while \(\vec{v}_i\) represents the average of the local velocity distribution of the background plasma ions. Thus, a fluid method is used to describe the background plasma while a kinetic description is employed for the impurity ions, since lower charge state impurities will not have sufficient time to thermalize to a Maxwellian velocity distribution before being ionized to a higher charge state.
A.5 Irreducible Hermite Polynomials

To find \( \eta(\vec{v}_i) \), Reiser adopted the method put forth by Balescu [12] of expanding \( \eta(\vec{v}_i) \) into a series of orthogonal polynomials—specifically Hermite polynomials since their weighting function is a Guassian, which coincides with the exponential of the Maxwellian velocity distribution \( f_0^0(\vec{v}_i) \). Due to anisotropies exhibited by the distribution function, Balescu then went further to select the irreducible-tensorial Hermite polynomials (further discussion on the selection and suitability of these polynomials is presented in the appendix of Balescu [12]).

\[
\eta(\vec{v}_i) = \sum_p h_p^{(3)} H_p^{(3)}(\vec{v}_i) + \sum_{p,q} h_{pq}^{(2)} H_{pq}^{(2)}(\vec{v}_i) \tag{A.18}
\]

where, using the polynomials from Abramowitz [16],

\[
H_p^{(3)}(\vec{v}_i) = \frac{1}{\sqrt{5}} \chi_p \left( 2\chi^2 - 5 \right) \tag{A.19}
\]

\[
H_{pq}^{(2)}(\vec{v}_i) = \sqrt{2} \left( \chi_p \chi_q - \frac{1}{3} \chi^2 \delta_{pq} \right) \tag{A.20}
\]

with the coefficients, \( h_p^{(3)} \) and \( h_{pq}^{(2)} \) having the very important physical interpretation

\[
h_p^{(3)} = \frac{2^{3/2}}{5} \left( \frac{m_i}{T_i} \right)^{3/2} \frac{1}{m_i n_i} q_p \tag{A.21}
\]

\[
h_{pq}^{(2)} = \frac{1}{\sqrt{2}} \frac{1}{n_i T_i} \pi_{pq} \tag{A.22}
\]

\( \pi_{pq} \) is the ion viscosity tensor and \( \vec{q} \) is the heat flux vector of the background plasma.

A.6 Imposition of Constraints

At this point it becomes important to note that numerical computations to plot the impurity trajectories are extremely time consuming when simulating the gyroscopic motion of the ion about the field line due to the Lorentz force appearing in (A.2). Therefore, Reiser has opted to transform \( C(f_s, f_i) \) into the drift-kinetic variables

\[ \vec{R} = \text{Guiding center position} \]
\( v_{\parallel} = \text{velocity parallel to the magnetic field} \)

\( v_{\perp} = \text{velocity perpendicular to the magnetic field} \)

to remove the dependency on the gyro-angle. Unfortunately, the general forms of the hermite coefficients, \( h_p \) and \( h_{pq} \), are not independent of the gyro-angle and therefore, Reiser imposed the following constraints:

1) The average background drift velocity will be directed parallel to the magnetic field line.

\[
\bar{v}_i \parallel \bar{b}, \quad \text{where} \quad \bar{b} = \frac{\bar{B}}{B}
\]

2) The general ion heat flux expression,

\[
\bar{q}_i = -\kappa_{\|} \nabla_{\|} T_i + \kappa_{\perp} \nabla_{\perp} T_i + \kappa_{\perp} \bar{b} \times \nabla_{\perp} T_i \quad \text{[17]}
\]

will also be reduced to being taken along the magnetic field line:

\[
\bar{q}_{\|} = -\kappa_{\|} \nabla_{\|} T_i
\]

where \( \kappa_{\|} = \frac{5}{2} \frac{n_i T_i \tau_{\|}}{m_i} \bar{\kappa}_{\|} \) is the thermal ion conductivity.

\[
\bar{\kappa}_{\|} = \frac{1}{0.5657}
\]

as obtained by Balescu [12] via the 13 moment approximation,

and where \( \tau_{\|} = \frac{3}{4} \left( \frac{4\pi e^2}{m_i} \right)^2 \frac{m_{1/2} T_{1/2}}{\sqrt{2\pi} n_i Z_i^4 e^{4\lambda}} \)

is the ion collision time for the background plasma.

3) Similarly, only the parallel ion viscosity tensor will be considered:

\[
\pi_{\parallel pq} = -\eta_{\parallel} \bar{v}_{\parallel pq},
\]

where the rate-of-strain tensor is

\[
\bar{V}_{\parallel} = \frac{1}{2} \begin{pmatrix}
2v_{xx} & 0 & 0 \\
0 & v_{yy} + v_{zz} & 0 \\
0 & 0 & v_{yy} + v_{zz}
\end{pmatrix}
\]
and the components are defined as \( \nu_{pp} = 2 \frac{\partial \nu_{ip}}{\partial x_p} - \frac{1}{3} \nabla \nu_i, \) \( \quad (A.31) \)

with the x-direction being parallel to \( \vec{B} \). Note that subscript 'i' in the components denotes 'ion' and does not represent an index.

\[ \eta_{ii} = n_i T_i \tau_i \eta_{ii} \] is the ion viscosity, \( \quad (A.32) \)

with \( \eta_{ii} = \frac{1}{1.2 + 0.8485 Z_i^{-1}} \) as given by Balescu [12]. \( \quad (A.33) \)

The net result of these constraints leads to

\[
h^{(3)}_{xx} = -\frac{3\sqrt{3}}{8\sqrt{\pi}} \frac{16 \pi^2 e_o^2}{Z_i^4 e^4} \frac{T_i}{n_i} \eta_{ii} \nabla_{\|} \nabla_{\parallel} \quad (A.34)
\]

\[
h^{(2)}_{xx} = -\frac{3}{8\sqrt{\pi}} \frac{16 \pi^2 e_o^2}{Z_i^4 e^4} \frac{T_i^{3/2}}{n_i} \eta_{ii} \left( -\frac{1}{3} \nabla \nu_i + 2 \nabla_{\|} \nu_{ii} \right) \quad (A.35)
\]

\[
h^{(2)}_{yy} = h^{(2)}_{zz} = -\frac{3}{8\sqrt{\pi}} \frac{16 \pi^2 e_o^2}{Z_i^4 e^4} \frac{T_i^{3/2}}{n_i} \eta_{ii} \left( \frac{2}{3} \nabla \nu_i - \nabla_{\|} \nu_{ii} \right) \quad (A.36)
\]

with all the remaining components of \( h^{(3)}_p \) and \( h^{(2)}_{pq} \) identically zero. We are now in a position to evaluate \( f_i(\bar{v}_i) \) and subsequently \( K_i \) and \( D_{ii} \).

### A.7 Evaluation of the Trubnikov Potentials

Let us summarize the steps so far. To evaluate the drift, \( K_i \) and diffusive, \( D_{ii} \), coefficients of \( (A.1) \), we need to evaluate the first and second order partial differential equations of the Trubnikov potentials, \( \phi_i(\bar{v}_i) \) and \( \psi_i(\bar{v}_i) \) respectively. To evaluate these potentials we need to know the velocity distribution function of the background plasma, \( f_i(\bar{v}_i) \). For an inhomogeneous background the function is taken to be a Maxwellian, \( f_i^0(\bar{v}_i) \), coupled with a small perturbation, \( \eta(\bar{v}_i) \):

\[
f_i(\bar{v}_i) = f_i^0(\bar{v}_i)(1 + \eta(\bar{v}_i)), \quad \text{where} \quad \eta(\bar{v}_i) = \sum_p h^{(3)}_p H^{(3)}_p(\bar{v}_i) + \sum_{p,q} h^{(2)}_{pq} H^{(2)}_{pq}(\bar{v}_i)
\]
with the irreducible Hermite polynomials, $H$, and their coefficients, $h$, as presented above, namely (A.19), (A.20) and (A.34), (A.35), and (A.36).

Remembering that $\Phi_1(\tilde{v}_z) = \int \frac{f_1(\bar{v}_i)}{|\bar{v}_z - \bar{v}_i|} d\bar{v}_i \quad \text{(A.37)}$

and $\Psi_1(\tilde{v}_z) = \int |\bar{v}_z - \bar{v}_i| f_1(\bar{v}_i) d\bar{v}_i, \quad \text{(A.38)}$

we can now move ahead and express the Trubnikov potentials in the following manner where the notation ‘I’ will be employed to represent the integrals:

\[
\begin{align*}
\Phi_1(\tilde{v}_z) &= \int \frac{f_1^0(\bar{v}_i)}{|\bar{v}_z - \bar{v}_i|} d\bar{v}_i + \sum_p h_p^{(3)} \int \frac{f_1^0(\bar{v}_i)H_p^{(3)}(\bar{v}_i)}{|\bar{v}_z - \bar{v}_i|} d\bar{v}_i + \sum_{p,q} h_{pq}^{(3)} \int \frac{f_1^0(\bar{v}_i)H_{pq}^{(3)}(\bar{v}_i)}{|\bar{v}_z - \bar{v}_i|} d\bar{v}_i \\
&=: I_1^1(\tilde{v}_z) \quad I_1^2(\tilde{v}_z) \quad I_1^{5}(\tilde{v}_z) \quad \text{(A.39)}
\end{align*}
\]

and similarly

\[
\begin{align*}
\Psi_1(\tilde{v}_z) &= \int |\bar{v}_z - \bar{v}_i| f_1^0(\bar{v}_i) d\bar{v}_i + \sum_p h_p^{(2)} \int |\bar{v}_z - \bar{v}_i| f_1^0(\bar{v}_i)H_p^{(2)}(\bar{v}_i) d\bar{v}_i \\
&+ \sum_{p,q} h_{pq}^{(2)} \int |\bar{v}_z - \bar{v}_i| f_1^0(\bar{v}_i)H_{pq}^{(2)}(\bar{v}_i) d\bar{v}_i \\
&=: I_2^1(\tilde{v}_z) \quad I_2^4(\tilde{v}_z) \quad I_2^{5}(\tilde{v}_z) \quad \text{(A.40)}
\end{align*}
\]

So,

\[
\begin{align*}
\Phi_1(\tilde{v}_z) &= I_1^1(\tilde{v}_z) + \sum_p h_p^{(3)} I_1^3(\tilde{v}_z) + \sum_{p,q} h_{pq}^{(3)} I_1^{5}(\tilde{v}_z) \\
&=: I_1(\tilde{v}_z) \quad \text{(A.41)}
\end{align*}
\]

\[
\begin{align*}
\Psi_1(\tilde{v}_z) &= I_2^1(\tilde{v}_z) + \sum_p h_p^{(2)} I_2^4(\tilde{v}_z) + \sum_{p,q} h_{pq}^{(2)} I_2^{5}(\tilde{v}_z) \\
&=: I_2(\tilde{v}_z) \quad \text{(A.42)}
\end{align*}
\]

The terms in the Trubnikov potentials represent the various kinds of interactions experienced by the impurity ion with the inhomogeneous, background plasma ions. Specifically, there are the drift terms:
\[
\phi_i(\bar{v}_z) = \int f_i^0(\bar{v}_i) \frac{d\bar{v}_i}{|\bar{v}_z - \bar{v}_i|} + \sum_p h_p^{(3)} \int f_i^0(\bar{v}_i) H_p^{(3)}(\bar{v}_i) \frac{d\bar{v}_i}{|\bar{v}_z - \bar{v}_i|} + \sum_{p,q} h_{pq}^{(3)} \int f_i^0(\bar{v}_i) H_{pq}^{(3)}(\bar{v}_i) \frac{d\bar{v}_i}{|\bar{v}_z - \bar{v}_i|}
\]

1\textsuperscript{st} term \hspace{5cm} 2\textsuperscript{nd} term \hspace{5cm} 3\textsuperscript{rd} term \hspace{5cm} (A.43)

- 1\textsuperscript{st} term represents the friction the impurity experiences with an unperturbed Maxwellian distribution of background ions.
- 2\textsuperscript{nd} term represents the friction the impurity experiences with a perturbed Maxwellian distribution arising from the variation in temperature of the background ions.
- 3\textsuperscript{rd} term represents the friction the impurity experiences with a perturbed Maxwellian distribution arising from the variation in bulk velocity of the background ions.

and the velocity diffusion terms:

\[
\psi_i(\bar{v}_z) = \int |\bar{v}_z - \bar{v}_i| f_i^0(\bar{v}_i) d\bar{v}_i + \sum_p h_p^{(2)} \int |\bar{v}_z - \bar{v}_i| f_i^0(\bar{v}_i) H_p^{(2)}(\bar{v}_i) d\bar{v}_i + \sum_{p,q} h_{pq}^{(2)} \int |\bar{v}_z - \bar{v}_i| f_i^0(\bar{v}_i) H_{pq}^{(2)}(\bar{v}_i) d\bar{v}_i
\]

1\textsuperscript{st} term \hspace{5cm} 2\textsuperscript{nd} term \hspace{5cm} 3\textsuperscript{rd} term \hspace{5cm} (A.44)

- 1\textsuperscript{st} term leads to diffusion of the impurity ion velocity under the effect of a pressure gradient arising from an unperturbed Maxwellian distribution of background ions.
- 2\textsuperscript{nd} term leads to diffusion of the impurity ion velocity under the effect of a temperature gradient within the background plasma (thermal velocity diffusion).
- 3\textsuperscript{rd} term leads to diffusion of the impurity ion velocity under the effect of a velocity gradient within the background plasma (viscous velocity diffusion).

We now proceed to evaluate the integrals of the Trubnikov potentials (A.39) and (A.40) using the relations.

\[
f_i^0 = \frac{\alpha^2}{\pi^{3/2}} e^{-\chi^2}; \quad d\bar{v}_i = \frac{d\bar{v}}{\alpha^2}; \quad \chi = \alpha(\bar{v}_z - \bar{v}_i); \quad \tilde{\omega} = \alpha(\bar{v}_z - \bar{v}_i); \quad |\bar{v}_z - \bar{v}_i| = \frac{1}{\alpha} |\bar{v} - \tilde{\omega}|
\]

(A.45)

where \( \bar{v}_z \) is the velocity of a single impurity ion, \( \bar{v}_z \) and \( \bar{v}_i \) are the average velocities of an ensemble of impurity and background plasma ions, respectively. The integrals are rewritten as
where $\delta_{pq}$ is the Dirac delta function. We now make the substitution $\vec{X} \rightarrow \vec{X} + \bar{\omega}$ and use the coordinate transformation,

$$
(\vec{X} + \bar{\omega})_p = \sum_j t_{pj}(\chi'_j + \omega'_j),
$$

(A.47)

to transform the components of the $\vec{X}$ and $\bar{\omega}$ to a coordinate system in which the $\bar{\omega}$ lies parallel to one of the axes:

$$
\omega'_p = \omega \delta_{pl} = \sum_j t_{pj}^{-1}\omega_j \quad \text{where } t_{pj}^{-1} \text{ is the transformation matrix.}
$$

(A.48)

The irreducible Hermite polynomial tensors, (A.19) and (A.20), transform accordingly:

$$
(\vec{X} + \bar{\omega})_p (2(\vec{X} + \bar{\omega})^2 - 5) = \sum_j t_{pj}(\chi'_j + \omega'_j)(2 \sum_n (\chi'_n + \omega'_n)^2 - 5)
$$

$$
(\vec{X} + \bar{\omega})_p (\vec{X} + \bar{\omega})_q - \frac{1}{3} (\vec{X} + \bar{\omega})^2 \delta_{pq} = \sum_{j,m} t_{pj}^{-1}t_{mq}^{-1}(\chi'_j + \omega'_j)(\chi'_m + \omega'_m) - \frac{1}{3} \sum_n (\chi'_n + \omega'_n)^2 \delta_{jm}
$$

(A.49)

A spherical coordinate system is employed to describe the velocity vectors in phase space:

$$
\chi'_1 + \omega'_1 = \chi \cos \theta + \omega \quad \chi'_2 + \omega'_2 = \chi \sin \theta \cos \phi \quad \chi'_3 + \omega'_3 = \chi \sin \theta \sin \phi
$$

(A.50)

$$
\delta \vec{X}' = \chi^2 \sin \theta d\theta d\phi d\chi
$$
Finally, the integrals of (A.46) can be expressed in terms of the integral,

\[ L_n = \int \int (x \sin \theta \cos \varphi)^n (x \cos \theta + \omega)^m \chi^* e^{-2x \cos \theta + \omega^2} \chi \sin \theta \sin \varphi \sin \chi \]  

(A.51)

where \( j, n, \) and \( m \) are integers with \( n,m \geq 0 \) and \( j = 0, \pm 1 \). Thus, (A.46) becomes

\[ \Gamma^1(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} L_{-1}^{00} \]

\[ \Gamma^2(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} L_{+1}^{00} \]

\[ \Gamma^3_p(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} \frac{1}{\sqrt{5}} t_{pl} (4L_{+i}^{21} + 3L_{+i}^{03} - 5L_{-i}^{01}) \]

\[ \Gamma^4_p(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} \frac{1}{\sqrt{5}} t_{pl} (4L_{+i}^{21} + 3L_{+i}^{03} - 5L_{-i}^{01}) \]

\[ \Gamma^5_{pq}(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} \sqrt{2} \left( \frac{2}{3} t_{pl} t_{lq} (L_{-1}^{02} - L_{-1}^{20}) - \frac{1}{3} t_{p2} t_{2q} (L_{-1}^{02} - L_{-1}^{20}) - \frac{1}{3} t_{p3} t_{3q} (L_{-1}^{20} - L_{-1}^{02}) \right) \]

\[ \Gamma^6_{pq}(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} \sqrt{2} \left( \frac{2}{3} t_{pl} t_{lq} (L_{+i}^{02} - L_{+i}^{20}) - \frac{1}{3} t_{p2} t_{2q} (L_{+i}^{02} - L_{+i}^{20}) - \frac{1}{3} t_{p3} t_{3q} (L_{+i}^{20} - L_{+i}^{02}) \right) \]

The following relations can be obtained from the definition of \( t_{pq} \):

\[ t_{pl} = \frac{\omega_p}{\omega}; \quad 2 t_{pl} t_{lq} - t_{p2} t_{2q} - t_{p3} t_{3q} = \frac{3}{\omega_p \omega_q} \delta_{pq} \]  

(A.53)

These are used to further reduce the last four integrals of (A.52):

\[ \Gamma^3_p(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} \frac{1}{\sqrt{5}} \frac{\omega_p}{\omega} (4L_{-1}^{21} + 2L_{-1}^{03} - 5L_{-1}^{01}) \]

\[ \Gamma^4_p(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} \frac{1}{\sqrt{5}} \frac{\omega_p}{\omega} (4L_{+i}^{21} + 2L_{+i}^{03} - 5L_{+i}^{01}) \]

\[ \Gamma^5_{pq}(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} \sqrt{2} \left( \frac{2}{3} \delta_{pq} - 3 \frac{\omega_p \omega_q}{\omega} \right) (L_{-1}^{02} - L_{-1}^{20}) \]

\[ \Gamma^6_{pq}(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} \sqrt{2} \left( \frac{2}{3} \delta_{pq} - 3 \frac{\omega_p \omega_q}{\omega} \right) (L_{+i}^{02} - L_{+i}^{20}) \]

(A.54)

All that remains is to evaluate the integral (A.51). Using the series expansion,
\[(y+x)^n = \sum_{k=0}^{n} \binom{n}{k} k y^{n-k}\]  \hspace{1cm} (A.55)

Integral (A.51) becomes

\[L_g^{2n-1} = \sum_{i=0}^{m} \int_{0}^{2\pi} \int_{0}^{\pi} \chi^{2n+m-i-g+2} \sin^{2n} \theta \cos^{m-i} \omega \cos^{2n} \phi \omega^{i} e^{-(\chi^2 + 2\chi \cos \theta + \omega^2)} \sin \theta d\theta d\phi d\chi\]

\[= \sum_{i=0}^{m} \int_{0}^{2\pi} \int_{0}^{\pi} \chi^{2n+m-i-g+2} (1-\cos^2 \theta)^n \cos^{m-i} \theta \cos^{2n} \phi \omega^{i} \]

\[\times e^{-(\chi^2 + 2\chi \cos \theta + \omega^2)} d\cos \theta d\phi d\chi\]

\[= 2\pi \left( \prod_{k=1}^{n} \frac{2k-1}{2k} \right) \sum_{i=0}^{m} \omega^{i} \sum_{j=0}^{\omega^{i}} (-1)^j \int_{0}^{\pi} \chi^{2n+m-i-g+2} \cos^{2j+m-i} \theta \]

\[\times e^{-(\chi^2 + 2\chi \cos \theta + \omega^2)} d\cos \theta d\chi\]  \hspace{1cm} (A.55)

Solving for \((1-\cos^2 \theta)^n:\)

\[L_g^{2n} = 2\pi \left( \prod_{k=1}^{n} \frac{2k-1}{2k} \right) \sum_{i=0}^{m} \omega^{i} \sum_{j=0}^{\omega^{i}} (-1)^j \int_{0}^{\pi} \chi^{2n+m-i-g+2} \cos^{2j+m-i} \theta \]

\[\times e^{-(\chi^2 + 2\chi \cos \theta + \omega^2)} d\cos \theta d\chi\]  \hspace{1cm} (A.57)

Using the formula,

\[\int x^n e^{-\beta x} dx = -\sum_{i=0}^{n} \frac{n!}{(n-i)!} \frac{x^{n-i}}{\beta^{i+1}} e^{-\beta x}\]  \hspace{1cm} (A.58)

and integrating over \(\theta,

\[L_g^{2n} = -2\pi \left( \prod_{k=1}^{n} \frac{2k-1}{2k} \right) \sum_{i=0}^{m} \omega^{i} \sum_{j=0}^{\omega^{i}} (-1)^j \int_{0}^{\pi} \chi^{2n+m-i-g+2} \cos^{2j+m-i} \theta \]

\[\times e^{-(\chi^2 + 2\chi \cos \theta + \omega^2)} d\cos \theta d\chi\]  \hspace{1cm} (A.59)
Making the substitution $\chi \to \chi \pm \omega$,

\[
L^m_n = -2\pi \sum_{k=1}^{n} \frac{2k-1}{2k} \omega^j \sum_{j=0}^{\infty} (-1)^j \sum_{p=0}^{2j+m-i-p} (2\omega)^{-p-1} \frac{(2j+m-i)!}{(2j+m-i-p)!} \int_{-\omega}^{\infty} (\chi - \omega)^{2n+m+g+1-i-p} e^{-\chi^2} d\chi - (-1)^{2j+m-i-p} \int_{-\omega}^{\infty} (\chi + \omega)^{2n+m+g+1-i-p} e^{-\chi^2} d\chi
\]

(A.60)

for which the final result becomes,

\[
L^m_n = -2\pi \sum_{k=1}^{n} \frac{2k-1}{2k} \omega^j \sum_{j=0}^{\infty} (-1)^j \sum_{p=0}^{2j+m-i-p} (2\omega)^{-p-1} \frac{(2j+m-i)!}{(2j+m-i-p)!} \int_{-\omega}^{\infty} (\sum_{s=0}^{q} \omega^j \int_{-\omega}^{\infty} (\chi - \omega)^{2n+m+g+1-i-p} \sum_{s=0}^{q} \omega^j \int_{-\omega}^{\infty} (\chi + \omega)^{2n+m+g+1-i-p} e^{-\chi^2} d\chi)
\]

(A.61)

where $q = 2n + m + g + 1 - i - p$. This final form of the integral allows one to actually evaluate all the terms of Trubnikov potentials, i.e. those of (A.52) and (A.54).

**A.7.1 Evaluation of the Trubnikov Potentials for an Unperturbed Maxwellian Distribution of Background Plasma Ions**

The complete evaluation of the Trubnikov Potentials will only be conducted for the simplest case for a Maxwellian distribution of plasma ions in the absence of any perturbations (i.e. no ion temperature or ion velocity gradients). This leads to the evaluation of the expressions corresponding to the first integrals of (A.39) and (A.40). Starting with the first integral of (A.39),

\[
I^1(\frac{\omega}{\pi^2}) = \frac{\alpha}{\pi^{3/2}} I^0_{-1}
\]

\[
= \frac{\alpha}{\pi^{3/2}} - \frac{2\pi}{2\omega} \int_{-\infty}^{\infty} e^{-\chi^2} d\chi - \int_{-\omega}^{\infty} e^{-\chi^2} d\chi
\]

\[
= \frac{\alpha}{\pi^{3/2}} - \frac{2\pi}{2\omega} \left( \int_{-\infty}^{\omega} e^{-\chi^2} d\chi - \int_{-\omega}^{\infty} e^{-\chi^2} d\chi - \int_{-\omega}^{\infty} e^{-\chi^2} d\chi - \int_{-\infty}^{\omega} e^{-\chi^2} d\chi \right)
\]

\[
= \frac{\alpha}{\pi^{3/2}} - \frac{2\pi}{2\omega} \left( \int_{-\omega}^{\omega} e^{-\chi^2} d\chi + \int_{-\omega}^{\omega} e^{-\chi^2} d\chi \right)
\]

(A.62)
Using the definition for the error function,

\[ \Phi(\omega) = \frac{2}{\sqrt{\pi}} \int_{0}^{\omega} e^{-x^2} \, dx \]  

(A.63)

with the property \( \Phi(-\omega) = -\Phi(\omega) \).

\[ I_1(\vec{v}_z) = \frac{\alpha}{\pi^{3/2}} \frac{2\pi}{2\omega} \left( 2\sqrt{\pi} - \frac{\Phi(\omega)}{\omega} \right) = \frac{\alpha}{\omega} \Phi(\omega) \]  

(A.64)

Regarding the first integral of (A.40),

\[ I_2(\vec{v}_z) = \frac{1}{\alpha \pi^{3/2}} \frac{2\pi}{2\omega} \left( \int_{\omega}^{\infty} (\chi - \omega)^2 e^{-\chi^2} \, d\chi - \int_{-\omega}^{\omega} (\chi + \omega)^2 e^{-\chi^2} \, d\chi \right) \]

\[ = \frac{1}{\alpha \pi^{3/2}} \frac{2\pi}{2\omega} \left( \int_{\omega}^{\infty} (\chi^2 - 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi - \int_{-\omega}^{\omega} (\chi^2 + 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi \right) \]

\[ = \frac{1}{\alpha \pi^{3/2}} \frac{2\pi}{2\omega} \left( -4\chi \omega e^{-\chi^2} \, d\chi - \int_{-\omega}^{\omega} (\chi^2 + 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi \right) \]  

(A.65)

The first integral in (A.65) becomes

\[ \int_{-\omega}^{\infty} -4\chi \omega e^{-\chi^2} \, d\chi = \int_{-\omega}^{0} -4\chi \omega e^{-\chi^2} \, d\chi - \int_{0}^{\infty} -4\chi \omega e^{-\chi^2} \, d\chi = -4\omega \left( \frac{1}{2} + \frac{1}{2} (e^{-\chi^2} - 1) \right) = -\omega \sqrt{\pi} \Phi'(\omega) \]  

(A.66)

where

\[ \Phi'(\omega) = \frac{2}{\sqrt{\pi}} e^{-\omega^2} \]  

(A.67)

is the derivative of the error function. The second integral in (A.65) becomes

\[ \int_{-\omega}^{\omega} (\chi^2 + 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi = \int_{-\omega}^{0} (\chi^2 + 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi + \int_{0}^{\infty} (\chi^2 + 2\chi \omega + \omega^2) e^{-\chi^2} \, d\chi \]  

(A.68)

where
Therefore,

\[
\int_0^\infty \chi^2 e^{-\chi^2} d\chi = \int_0^\infty \chi^2 e^{-\chi^2} d\chi = -\frac{1}{2} \left( \omega e^{-\chi^2} - \int_0^\infty e^{-\chi^2} d\chi \right) = -\frac{\sqrt{\pi}}{4} \left( \Phi(\omega) - \omega \Phi'(\omega) \right)
\]

\[
\int_0^\infty 2\omega e^{-\chi^2} d\chi = -\int_0^\infty 2\omega e^{-\chi^2} d\chi = \omega(e^{-\chi^2} - 1)
\]

Therefore,

\[
I^2(\bar{v}_z) = \frac{1}{\alpha} \sqrt{\frac{\pi}{2}} \left[ -\omega \sqrt{\pi} \Phi'(\omega) - \frac{\sqrt{\pi}}{2} \left( \Phi(\omega) - \omega \Phi'(\omega) \right) - \omega^2 \sqrt{\pi} \Phi(\omega) \right]
\]

\[
= \frac{1}{2\alpha} \Phi'(\omega) + \left( \frac{1}{2\alpha \omega} + \frac{\omega}{\alpha} \right) \Phi(\omega)
\]

Finally, \( \frac{\partial}{\partial \omega} I^1(\bar{v}_z) \) and \( \frac{\partial^2}{\partial \omega^2} I^2(\bar{v}_z) \) correspond to the Spitzer coefficients [4],

\[
\frac{d}{dt} \langle \Delta v_{all} \rangle \quad \text{and} \quad \frac{d}{dt} \langle (\Delta v_{all})^2 \rangle,
\]

introduced in chapter 1 when \( \omega < 1 \).

**A.7.2 The Trubnikov Potentials Including the Effects of Ion Temperature and Ion Velocity Gradients**

The terms of the potentials involving the ion temperature and ion velocity gradients will not be explicitly evaluated, only their final results are will be listed below. Also, \( \omega \) represents the difference between the average speed of an ensemble of impurity ions and the average speed of the background plasma ions. In a Monte Carlo simulation each impurity ion is treated individually and therefore \( \omega \) will be replaced by \( \chi \) where \( \chi \) is the difference in speed of a single impurity ion with respect to the average speed of the background plasma flow. Therefore, the integrals of (A.39) and (A.40) are

\[
I^1(\bar{v}_z) = \frac{\alpha}{\chi} \Phi(\chi)
\]

\[
\Phi_0(\chi)
\]
\[ I^2(\vec{v}_z) = \frac{1}{2\alpha} \Phi(\chi) + \left( \frac{1}{2\alpha} + \frac{1}{\alpha} \right) \Phi(\chi) \]  
\[ \psi_0(\chi) \]  
\[ I^3_\perp(\vec{v}_z) = -\frac{1}{\sqrt{5}} \frac{X_p}{\chi^2} \alpha \chi \Phi(\chi) \]  
\[ \phi_1(\chi) \]  
\[ I^4_\perp(\vec{v}_z) = -\frac{1}{\sqrt{5}} \frac{X_p}{\chi^2} \frac{\Phi(\chi)}{2\alpha^2} - \frac{1}{2\alpha^2} \Phi(\chi) \] 
\[ \psi_1(\chi) \]  
\[ I^5_{\perp q}(\vec{v}_z) = \frac{1}{2\sqrt{2}} \left( \delta_{pq} - 3 \frac{X_pX_q}{\chi^2} \right) \left[ \left( \frac{2\alpha}{3} + \frac{\alpha}{\chi^2} \right) \Phi(\chi) - \frac{\alpha}{\chi^2} \Phi(\chi) \right] \] 
\[ \phi_2(\chi) \]  
\[ I^6_{\perp q}(\vec{v}_z) = \frac{1}{2\sqrt{2}} \left( \delta_{pq} - 3 \frac{X_pX_q}{\chi^2} \right) \left[ \frac{1}{2\alpha^2} \Phi(\chi) + \left( \frac{1}{3\alpha} - \frac{1}{2\alpha^3} \right) \Phi(\chi) \right] \] 
\[ \psi_2(\chi) \]  

where \( \phi_i \rightarrow \phi \) and \( \psi_i \rightarrow \psi \) are used as a notation simplification. For the summations appearing in (A.41) and (A.42), the only nonzero terms involve \( h^{(3)}_x \), \( h^{(2)}_{xx} \), \( h^{(2)}_{yy} \), and \( h^{(2)}_{zz} \), with \( x \)-direction being along the field line. Additionally, \( h^{(2)}_{yy} = h^{(2)}_{zz} \) and

\[ \chi^2 = \chi^2_{il} + \chi^2_{l\perp}, \quad \chi^2_{l\perp} = \chi^2_y + \chi^2_z, \quad \chi^2_{il} = \chi^2_x \]  
\[ (A.77) \]

This then leads to the final result for the Trubnikov potentials:

\[ \Phi(\vec{v}_z) = \phi_0(\chi) + \left( -\frac{h^{(3)}_x}{\sqrt{5}} \right) \chi \phi_1(\chi) + \frac{1}{2\sqrt{2}} \left( h^{(2)}_{xx} - \frac{1}{2} \left( h^{(2)}_{yy} + h^{(2)}_{zz} \right) \right) \left( 1 - \frac{3\chi^2}{\chi^2} \right) \phi_2(\chi) \]  
\[ (A.78) \]
In order to evaluate the drift and diffusive coefficients in terms of directions parallel and perpendicular to the magnetic field lines (i.e. $K_\parallel$ and $K_\perp$ rather than $K_x$, $K_y$, $K_z$) it is necessary to transform the velocity components from Cartesian $(v_x, v_y, v_z)$ to drift-kinetic variables $(v_\parallel, v_\perp, \theta_B)$. Reiser this accomplishes by applying the methodology of tensor analysis to the collision term $C(f_\parallel, f_\perp)$ to convert it to the new reference frame. Using Christofel symbols of the first and second order, the partial derivatives depending on the gyration angle about the field line, $\theta_B$, are effectively eliminated. The details of the transformation are given in his thesis [5].

The full set of components of (A.4) and (A.5) in the new reference frame are consequently of the form

$$K_\parallel = \left(1 + \frac{m_2}{m_i}\right) \Lambda \frac{\partial \phi}{\partial v_\parallel}; \quad K_\perp = \left(1 + \frac{m_2}{m_i}\right) \Lambda \frac{\partial \psi}{\partial v_\perp} + \frac{\Lambda}{2} \frac{1}{v_\perp^2} \frac{\partial \psi}{\partial v_\perp}$$

$$D_{\parallel\parallel} = \Lambda \frac{\partial^2 \psi}{\partial v_\parallel^2}; \quad D_{\parallel\perp} = \Lambda \frac{\partial^2 \psi}{\partial v_\parallel \partial v_\perp}; \quad D_{\perp\parallel} = \Lambda \frac{\partial^2 \psi}{\partial v_\perp \partial v_\parallel}; \quad D_{\perp\perp} = \Lambda \frac{\partial^2 \psi}{\partial v_\perp^2}$$

The first order partial derivative of $\phi$ and the second order partial derivative of $\psi$ with respect to $\chi$ are

$$\frac{\partial \phi_\parallel(\chi)}{\partial \chi} = \frac{\alpha}{\chi} \Phi'(\chi) - \frac{\alpha}{\chi^2} \Phi(\chi)$$

$$\frac{\partial \phi_\perp(\chi)}{\partial \chi} = (\alpha - 2\alpha \chi^2) \Phi'(\chi)$$

$$\frac{\partial \phi_\parallel(\chi)}{\partial \chi} = \left(\frac{4\alpha \chi}{3} + \frac{2\alpha}{\chi} + \frac{3\alpha}{\chi^3}\right) \Phi'(\chi) + \frac{3\alpha}{\chi^4} \Phi(\chi)$$
and

$$\frac{\partial^2 \psi_o(\chi)}{\partial \chi^2} = -\frac{1}{\alpha \chi^2} \Phi'(\chi) + \frac{1}{\alpha \chi^3} \Phi(\chi)$$  \hspace{1cm} (A.86)

$$\frac{\partial^2 \psi_1(\chi)}{\partial \chi^2} = \left( \frac{2 \chi}{\alpha} + \frac{2}{\alpha \chi} + \frac{3}{\alpha \chi^3} \right) \Phi'(\chi) - \frac{3}{\alpha \chi^4} \Phi(\chi)$$  \hspace{1cm} (A.87)

$$\frac{\partial^2 \psi_2(\chi)}{\partial \chi^2} = \left( \frac{4}{3 \alpha} + \frac{10}{3 \alpha \chi^2} + \frac{6}{\alpha \chi^4} \right) \Phi'(\chi) + \left( \frac{2}{3 \alpha \chi^3} - \frac{6}{\alpha \chi^5} \right) \Phi(\chi)$$  \hspace{1cm} (A.88)

Since we are only interested in the parallel-to-B motion, $\chi_\parallel$ is set to 0. The first order partial derivative of $\Phi$ and the second order partial derivative of $\psi$ with respect to $v_{z\parallel}$ are easily evaluated since

$$\frac{\partial \Phi(\chi)}{\partial v_{z\parallel}} = \Phi'(\chi) \frac{\partial \chi}{\partial v_{z\parallel}}$$ \hspace{1cm} and \hspace{1cm} $$\frac{\partial \Phi'(\chi)}{\partial v_{z\parallel}} = -2\chi \Phi'(\chi) \frac{\partial \chi}{\partial v_{z\parallel}}$$

where

$$\chi_\parallel = \alpha (\bar{v}_{z\parallel} - \bar{v}_{\parallel}) \hspace{1cm} and \hspace{1cm} \chi = \sqrt{\chi_\parallel^2 + \chi_\perp^2} \hspace{1cm} such \hspace{1cm} that \hspace{1cm} \frac{\partial \chi_\parallel}{\partial v_{z\parallel}} = \alpha \hspace{1cm} and \hspace{1cm} \frac{\partial \chi}{\partial v_{z\parallel}} = \alpha \frac{\chi_\parallel}{\chi}$$

Note that the subscript 'z' denotes 'impurity of charge Z' and does not represent motion that is strictly along the z-axis. Therefore,

$$\frac{\partial \phi}{\partial v_{z\parallel}} = \frac{\chi_\parallel}{\chi} \left( \frac{\partial \Phi_o}{\partial \chi} + C_1 \frac{\chi_\parallel}{\chi} \frac{\partial \Phi_1}{\partial \chi} + C_2 \left( 1 - 3 \frac{\chi_\parallel^2}{\chi^2} \right) \frac{\partial \Phi_2}{\partial \chi} \right)$$  \hspace{1cm} (A.89)

$$\frac{\partial^2 \psi}{\partial v_{z\parallel}^2} = \alpha^2 \frac{\chi_\parallel^2}{\chi^2} \left( \frac{\partial^2 \psi_0}{\partial \chi^2} + C_1 \frac{\chi_\parallel}{\chi} \frac{\partial^2 \psi_1}{\partial \chi^2} + C_2 \left( 1 - 3 \frac{\chi_\parallel^2}{\chi^2} \right) \frac{\partial^2 \psi_2}{\partial \chi^2} \right)$$  \hspace{1cm} (A.90)

We now have the complete form of the parallel drift and diffusive coefficients

$$K_{\parallel} = \left( 1 + \frac{m_\parallel}{m_i} \right) \alpha \frac{\chi_\parallel}{\chi} \left( \phi_o' + C_1 \frac{\chi_\parallel}{\chi} \phi_1' + C_2 \left( 1 - 3 \frac{\chi_\parallel^2}{\chi^2} \right) \phi_2' \right)$$  \hspace{1cm} (A.91)
\[ D_{\parallel \parallel} = \Lambda \alpha^2 \frac{\chi_\parallel^2}{\chi^2} \left( \psi_\parallel^* + C_1 \frac{\chi_\parallel}{\chi} \psi_\parallel^* + C_2 \left( 1 - 3 \frac{\chi_\parallel^2}{\chi^2} \right) \psi_\parallel^* \right) \]  
(A.92)

where \( \phi^* = \frac{\partial \phi}{\partial \chi} \) and \( \psi^* = \frac{\partial^2 \psi}{\partial \chi^2} \)

### A.9 Further Simplification of the Drift and Diffusive Coefficients:

\( K_\parallel \) and \( D_{\parallel \parallel} \) can be rewritten in three component form

\[ K_\parallel = K_\parallel (\phi_0') + K_\parallel (\phi_1') + K_\parallel (\phi_2') \]  
(A.93)

\[ D_{\parallel \parallel} = D_{\parallel \parallel} (\psi_0^* ) + D_{\parallel \parallel} (\psi_1^* ) + D_{\parallel \parallel} (\psi_2^* ) \]  
(A.94)

Since \( \chi_\perp = 0 \) and \( \chi^2 = \chi_\parallel^2 \left( 1 - 3 \frac{\chi_\parallel^2}{\chi^2} \right) \) simplifies to \(-2\) in (A.91) and (A.92) so

\[ K_\parallel (\phi_0') = K_\parallel (n_i) = \left( 1 + \frac{m_1}{m_i} \right) \Lambda \alpha^2 \frac{\chi_\parallel}{\chi} \left( \frac{\Phi'(\chi)}{\chi} - \frac{\Phi(\chi)}{\chi^2} \right) \]  
(A.95)

\[ K_\parallel (\phi_1') = K_\parallel (V_1 T_1) = \left( 1 + \frac{m_1}{m_i} \right) \Lambda \alpha^2 C_1 \left( 1 + 2 \frac{\chi_\parallel}{\chi} \right) \Phi'(\chi) \]  
(A.96)

\[ K_\parallel (\phi_2') = K_\parallel (V_\parallel V_\parallel) = \left( 1 + \frac{m_1}{m_i} \right) \Lambda \alpha^2 2 C_2 \frac{\chi_\parallel}{\chi} \left( \frac{4}{3} \frac{\chi}{\chi^3} + \frac{2}{3} \frac{2}{\chi^3} \right) \Phi'(\chi) \left( 1 - \frac{3}{\chi^4} \Phi(\chi) \right) \]  
(A.97)

and

\[ D_{\parallel \parallel} (\psi_0^* ) = D_{\parallel \parallel} (n_i) = \Lambda \alpha \frac{\chi_\parallel^2}{\chi^2} \left( \frac{\Phi(\chi)}{\chi^3} - \frac{\Phi'(\chi)}{\chi^2} \right) \]  
(A.98)

\[ D_{\parallel \parallel} (\psi_1^* ) = D_{\parallel \parallel} (V_1 T_1) = \Lambda \alpha C_1 \frac{\chi_\parallel^2}{\chi^2} \left[ \left( 2 \frac{\chi}{\chi^3} + \frac{3}{3} \frac{2}{\chi^3} \right) \Phi'(\chi) - \frac{3}{\chi^4} \Phi(\chi) \right] \]  
(A.99)

\[ D_{\parallel \parallel} (\psi_2^* ) = D_{\parallel \parallel} (V_\parallel V_\parallel) = -2 \Lambda \alpha C_2 \frac{\chi_\parallel^2}{\chi^2} \left[ \left( \frac{4}{3} + \frac{10}{3} \frac{2}{\chi^2} + \frac{6}{\chi^4} \right) \Phi'(\chi) + \left( \frac{2}{3} \frac{2}{\chi^2} - \frac{6}{\chi^5} \right) \Phi(\chi) \right] \]  
(A.100)
where the $\chi_{\perp}^2$ term has been retained in $D_{\parallel\parallel}$ for completeness even though it equals 1 when $\chi_{\perp} = 0$. Each of the drift terms can be further expanded to show more clearly the dependence on the background quantities:

\[
K_{\parallel}(n_i) = \left(1 + \frac{m_i}{m_z}\right) \frac{\chi_{\parallel}^2 m_i}{4\pi \varepsilon_0^2 m_z} n_i \chi_{\parallel}^2 \left(\frac{\Phi(\chi) - \chi'\Phi'(\chi)}{2\chi^2}\right)
\]

(A.101)

\[
K_{\parallel}(\nabla_{\parallel} T_i) = \left(1 + \frac{m_i}{m_z}\right) \frac{3\chi_{\parallel}^2}{2Z_i^2 m_z} \bar{n}_{\parallel} (1 - 2\chi_{\parallel}^2) \exp(-\chi^2) \nabla_{\parallel} T_i
\]

(A.102)

\[
K_{\parallel}(\nabla_{\parallel} v_{\parallel\parallel}) = -\left(1 + \frac{m_i}{m_z}\right) \frac{3\chi_{\parallel}^2}{2Z_i^2 m_z} \bar{n}_{\parallel} \left[\frac{2}{\chi^2} \left(\frac{\Phi(\chi)}{\chi^2} - \frac{3}{\chi^4} \Phi'(\chi)\right)\right] \nabla_{\parallel} v_{\parallel\parallel}
\]

(A.103)

where, by neglecting the perpendicular motion, $\nabla v_i = \nabla_{\parallel} v_{\parallel\parallel}$ in the $C_i$ coefficient. Also, we have explicitly represented $\Phi'(\chi)$ as $\frac{2}{\sqrt{\pi}} \exp(-\chi^2)$ in the $K_{\parallel}(\nabla_{\parallel} T_i)$ term. Similarly for the diffusion terms one has

\[
D_{\parallel\parallel}(n_i) = \frac{\chi_{\parallel}^2}{4\pi \varepsilon_0^2 m_z} \bar{n}_{\parallel} \sqrt{\frac{m_i}{2T_i}} \chi_{\parallel}^2 \left(\frac{\Phi(\chi) - \chi'\Phi'(\chi)}{2\chi^2}\right)
\]

(A.104)

\[
D_{\parallel\parallel}(\nabla_{\parallel} T_i) = \frac{3\chi_{\parallel}^2}{2Z_i^2 m_z} \bar{n}_{\parallel} \left[\frac{2}{\chi^2} \left(\frac{\Phi(\chi)}{\chi^2} - \frac{3}{\chi^4} \Phi'(\chi)\right)\right] \nabla_{\parallel} T_i
\]

(A.105)

\[
D_{\parallel\parallel}(\nabla_{\parallel} v_{\parallel\parallel}) = \sqrt{\pi} \frac{3\chi_{\parallel}^2}{2Z_i^2 m_z} \bar{n}_{\parallel} \chi_{\parallel}^2 \left[\frac{4}{3} + \frac{10}{3} \frac{6}{\chi^4} \Phi'(\chi) + \left(\frac{2}{3} - \frac{6}{\chi^5}\right) \Phi(\chi)\right] \nabla_{\parallel} v_{\parallel\parallel}
\]

(A.106)

These then are the final forms of the drift and diffusive coefficients for an impurity ion moving parallel to the magnetic field.
Appendix B: Limits of the Temperature and Velocity Gradients of the Background Plasma when using the Drift-Kinetic Model

As stated in Reiser's Ph.D. thesis [5], using a Maxwellian distribution function with a small perturbation to describe the background plasma (see Appendix A.4) allows one to use a fluid analysis to solve the kinetic equation for an impurity ion interacting with the background plasma. The perturbation represents the effects on the impurity of the temperature and velocity gradients of the background plasma. However, as originally stated by Braginskii [8], the effects arising from these gradients are defined under the assumption that the relaxation process which forces the distribution function to approach a Maxwellian is not inhibited. This requires that all averaged background quantities change slowly in time and space. As such, the mean free path between collisions must be smaller than the gradient scale length. A means of determining the minimum gradient scale length for the drift-kinetic model is presented below.

The full set of drift (A.81) and diffusive (A.82) coefficients provide a complete description of the impurity ion motion in the parallel and perpendicular-to-B directions. With these coefficients the drift-kinetic equation (A.2) is represented as

$$\frac{\partial f_z(\vec{v})}{\partial t} = \sum_i C_{zi}(f_z(\vec{v}), f_i(\vec{v}))$$

(B.1)

where

$$\frac{\partial f_z(\vec{v})}{\partial t} = -\frac{\partial}{\partial \vec{v}_\parallel} \left( K_z f_z(\vec{v}) \right) - \frac{\partial}{\partial \vec{v}_\perp} \left( K_\perp f_z(\vec{v}) \right) + \frac{1}{2} \frac{\partial^2}{\partial \vec{v}_\parallel^2} \left( D_{\parallel \parallel} f_z(\vec{v}) \right) + \frac{1}{2} \frac{\partial^2}{\partial \vec{v}_\parallel \partial \vec{v}_\perp} \left( D_{\parallel \perp} f_z(\vec{v}) \right)$$

$$+ \frac{1}{2} \frac{\partial^2}{\partial \vec{v}_\perp \partial \vec{v}_\perp} \left( D_{\perp \perp} f_z(\vec{v}) \right)$$

(B.2)

The diffusive terms $D_{\parallel \parallel}$, $D_{\parallel \perp}$, $D_{\perp \parallel}$, and $D_{\perp \perp}$ are the components of a diffusion tensor. To prevent the possibility of the distribution function $f_z(\vec{v})$ from becoming negative, the diffusion tensor must be positive semi-definite [14]. More precisely, if one takes the point $\vec{v} = \vec{v}_0$ to be the location where $f_z(\vec{v})$ equals 0 (i.e. a local minimum), it follows that for a small distance from that point, $1 \cdot |\vec{v} - \vec{v}_0| \cdot f_z(\vec{v})$ must be positive,

$$f_z(\vec{v}) = \frac{1}{2} \sum_{p,q} \frac{\partial^2 f(\vec{v})}{\partial v_p \partial v_q} (v_p - v_{0p})(v_q - v_{0q}) > 0 \text{ when } \vec{v} = \vec{v}_0$$

(B.3)
This implies that when $\bar{v} = \bar{v}_0$, the tensor $\frac{\partial^2 f_z(\bar{v})}{\partial v_p \partial v_q}$ must be positive definite (Note: the indices p and q index through the $\parallel$ and $\perp$ directions). Evaluating the drift-kinetic equation (B.2) at the point where $\bar{v} = \bar{v}_0$ results in

$$\frac{\partial f_z(\bar{v})}{\partial t} = \frac{1}{2} \sum_{p,q} D_{pq} \frac{\partial^2 f_z(\bar{v})}{\partial v_p \partial v_q} \text{ when } \bar{v} = \bar{v}_0$$ (B.4)

Therefore, to ensure $\frac{\partial f_z(\bar{v})}{\partial t} \geq 0$ when $\bar{v} = \bar{v}_0$, the diffusion tensor $D_{pq}$ must be positive semi-definite. For this to be true, the determinant of the symmetric matrix $D_{pq}$ must be greater than or equal to zero for all values of $\bar{v}$. The matrix components are represented as

$$D_{pq} = \Lambda \frac{\partial^2 \psi_1(\bar{v}_z)}{\partial v_p \partial v_q}$$ (B.5)

where $\psi_1(\bar{v}_z)$ is one of the Trubnikov potentials (A.9). The matrix itself can be represented as

$$\Lambda \begin{pmatrix} \frac{\partial^2 \psi}{\partial v^2} & \frac{\partial^2 \psi}{\partial v \partial \bar{v}} \\ \frac{\partial^2 \psi}{\partial \bar{v} \partial v} & \frac{\partial^2 \psi}{\partial \bar{v}^2} \end{pmatrix} = \Lambda \frac{\alpha^2}{\chi^2} \begin{pmatrix} \chi_{\parallel} & -\chi_{\perp} \\ -\chi_{\perp} & \chi_{\parallel} \end{pmatrix} \begin{pmatrix} \bar{C}_0 + C_1 \bar{C}_1 + C_2 \bar{C}_2 \end{pmatrix} \begin{pmatrix} \chi_{\parallel} & \chi_{\perp} \\ -\chi_{\perp} & \chi_{\parallel} \end{pmatrix}$$ (B.6)

with

$$\bar{C}_0 = \begin{pmatrix} \psi_0' & 0 \\ 0 & \psi_0' \end{pmatrix}, \quad \bar{C}_1 = \begin{pmatrix} \chi_{\parallel} & -\chi_{\perp} \\ -\chi_{\perp} & \chi_{\parallel} \end{pmatrix} \begin{pmatrix} \psi_1' & \psi_1' \\ \psi_1' & \psi_1' \end{pmatrix}$$

$$\bar{C}_2 = \begin{pmatrix} \frac{1-3 \chi_{\parallel}^2}{\chi^2} \psi_2' \\ \frac{6 \chi_{\parallel} \chi_{\perp} \psi_2' - \psi_2'}{\chi^2} \\ \frac{6 \chi_{\parallel} \chi_{\perp} \psi_2' - \psi_2'}{\chi^2} \end{pmatrix}$$

$\bar{C}_0$ corresponds to that part of the diffusion tensor, which describes the interaction of the impurity ion with the unperturbed Maxwellian distribution of the background plasma. $\bar{C}_1$ corresponds to
the perturbation arising from the presence of a temperature gradient while $\overline{C}_2$ corresponds to the perturbation arising from a velocity gradient. Using the requirement that the diffusion tensor be positive semi-definite one can determine the values of the constants $C_1$ and $C_2$ in (B.6) which in turn can be used to set the limits of the values for the temperature and velocity gradient scale lengths of the background plasma.

The constants $C_1$ and $C_2$ are functions of the coefficients $h^{(3)}_x$ (A.34), $h^{(2)}_{xx}$ (A.35), $h^{(2)}_{yy}$ (A.36), and $h^{(2)}_{zz}$ (A.36) of the irreducible Hermite polynomials:

$$C_1 = -\frac{h^{(3)}_x}{\sqrt{5}}$$

$$C_2 = \frac{1}{2\sqrt{2}} \left( \frac{h^{(2)}_{xx} - \frac{1}{2}(h^{(2)}_{yy} + h^{(2)}_{zz})}{2\sqrt{2}} \right)$$

(B.8)

Rewritten in terms of the physical quantities that define the coefficients:

$$C_1 = \frac{6\pi^2 e_0^2}{\sqrt{\pi Z_i^4 e^4 \lambda}} \frac{T_i}{n_i} \frac{1}{\nabla_i T_i}$$

(B.9)

$$C_2 = \frac{3\pi^2 e_0^2}{\sqrt{2\pi Z_i^4 e^4 \lambda}} \frac{m_i^{1/2} T_i^{3/2}}{n_i} \left( \frac{1}{3} \nabla_i^2 - 3 \nabla_i v_{\parallel} \right)$$

(B.10)

(B.9) can be re-expressed in terms of the temperature gradient scale length,

$$\frac{T_i}{\nabla_i T_i} = \frac{6\pi^2 e_0^2}{\sqrt{\pi Z_i^4 e^4 \lambda}} \frac{T_i^2}{n_i}$$

(B.11)

while (B.10) can be re-expressed in terms of the velocity gradient scale length,

$$\frac{v_{th}}{2\nabla_i v_{\parallel}} = \frac{3\pi^2 e_0^2}{\sqrt{2\pi Z_i^4 e^4 \lambda}} \frac{T_i^2}{n_i}$$

(B.12)

where $v_{th} = \sqrt{2T_i/m_i}$ and $\left( \nabla_i v_i - 3 \nabla_i v_{\parallel} \right) = -2 \nabla_i v_{\parallel}$ since only the parallel-to-B velocity components are being considered (i.e. $\nabla_i v_i = \nabla_i v_{\parallel}$). To obtain a minimum value for (B.11) and (B.12), appropriate values for $C_1$ and $C_2$ must be provided. The requirement that the diffusion tensor be positive semi-definite means that the determinant of the matrix on the left hand side of (B.6) must be greater than or equal to zero. Considering for the moment only the effect of the temperature gradient, one can represent this requirement in terms of the right hand side of (B.6) as
where \( a_1, b_1, c_1 \) are evaluated in terms of the matrix components of \( \overline{C}_0 \) and \( \overline{C}_1 \):

\[
det(\overline{C}_0 + C_1 \overline{C}_1) = a_1 + b_1 C_1 + c_1 C_1^2 \geq 0
\]  \hspace{1cm} (B.13)

The values of \( C_1 \) can then be determined by finding the roots of the polynomial in (B.13):

\[
C_1^2 = -\frac{b_1 \pm \sqrt{b_1^2 - 4a_1c_1}}{2c_1}
\]  \hspace{1cm} (B.15)

Figure 48a shows the values of the inverses of \( C_1^+ \) and \( C_1^- \) for various values of \( \chi = b \chi_\perp \) (\( \chi_\perp = 0 \)). Two sets of curves for \( 1/C_1^+ \) and \( 1/C_1^- \) are displayed corresponding to positive and negative values of \( \chi_\perp \). The region between a given pair of \( 1/C_1^+ \) and \( 1/C_1^- \) values represent values for which the DK model is no longer valid. Thus the largest value of \( 1/C_1 \) will ensure the validity of the DK model for all possible impurity ion velocities (as represented by \( \chi \)). This value for \( 1/C_1 \) provides the largest minimum value for the temperature gradient scale length. From the figure, the largest value of \( 1/C_1 \) is approximately 1 when \( \chi \) is 2.75. Therefore, with this value of \( C_1 \), one obtains the criterion from (B.11)

\[
L_{\text{Ti}} = \frac{T_i}{|V_{\text{Ni}}|} \geq L_{\text{min}}^{\text{Ti}} = 4 \times 10^{-54} \frac{\bar{\nu} T_i^2}{\lambda Z_i^4 n_i}
\]  \hspace{1cm} (B.16)

where \( L \) is in m, \( v \) is in m/s, \( T \) is in J, and \( n_i \) is in m\(^{-3}\). This assures that \( f_\perp (\bar{v}) \geq 0 \) for all values of the relative velocity between the impurity ion and the background plasma ions.

The criterion for the velocity gradient scale lengths is determined similarly. This time, only the effect of the velocity gradient is considered such that the requirement for the determinant of
the right hand side of (B.6) is now expressed as

\[
\det(\overline{C}_0 + C_2 \overline{C}_2) = a_2 + b_2 C_2 + c_2 C_2^2 \geq 0
\]  

(B.17)

where \(a_2, b_2, \) and \(c_2\) are evaluated from the components of \(\overline{C}_0\) and \(\overline{C}_2\):

\[
a_2 = \psi_0^* (\chi) \frac{\psi_0' (\chi)}{\chi}
\]  

(B.18)

\[
b_2 = \left(1 - 3 \frac{\chi_i^2}{\chi^2}\right) \psi_0^* (\chi) \frac{\psi_2 (\chi)}{\chi} - 6 \left(1 - 2 \frac{\chi_i^2}{\chi^2}\right) \psi_0^* (\chi) \frac{\psi_2 (\chi)}{\chi^2} + \left(1 - 3 \frac{\chi_i^2}{\chi^2}\right) \psi_2^* (\chi) \frac{\psi_0 (\chi)}{\chi}
\]

\[
c_2 = \left(1 - 3 \frac{\chi_i^2}{\chi^2}\right)^2 \psi_2^* (\chi) \frac{\psi_2 (\chi)}{\chi} - 6 \left(1 - 3 \frac{\chi_i^2}{\chi^2}\right) \left(1 - 2 \frac{\chi_i^2}{\chi^2}\right) \psi_2^* (\chi) \frac{\psi_2 (\chi)}{\chi^2} - 36 \frac{\chi_i^2 \chi_i^4}{\chi} \left(\frac{\psi_2 (\chi)}{\chi} - \frac{\psi_2^* (\chi)}{\chi}\right)^2
\]

The values of \(C_2\) are also determined by finding the roots of the polynomial in (B.17):

\[
C_2^\pm = -\frac{b_2 \pm \sqrt{b_2^2 - 4a_2c_2}}{2c_2}
\]  

(B.19)

Figure 48b shows the profiles of \(1/C_2^+\) and \(1/C_2^-\) for various values of \(\chi\). The maximum value of \(1/C_2\) occurs when \(\chi\) is extremely large. Nevertheless, taking 1.25 as the maximum value means \(C_2 = 0.8\), providing the following criterion from (B.12):

\[
L_{vi} = \frac{v_{th}}{2V_i^\|} \geq L_{vi}^{\min} = 2.7 \times 10^{54} \frac{\bar{T}_i^2}{\lambda Z_i n_i}
\]  

(B.20)

again, \(L\) is in m, \(v\) is in m/s, \(T\) is in J, and \(n_i\) is in m\(^3\).

It is therefore necessary to evaluate the temperature and the velocity gradient scale lengths for each grid cell in the SOL and the private plasma and to compare them to the minimum values calculated from the quantities of \(T_i, n_i,\) and \(Z_i\) for that cell (note: \(\lambda\) is the Coulomb logarithm = 15, \(\bar{\kappa}_i\) is the thermal ion conductivity = 1/0.5657, and \(\bar{\eta}_i\) is the ion viscosity = 1/(1.2 + 0.8485Z_i\(^{-1}\)).

In those regions where the gradient scale lengths are smaller than the minimum value, the DK model is no longer valid in describing the motion of impurity ions.
Appendix C: Derivation of the Trubnikov Potentials showing their Dependency on the Coulomb Cross Section

The following is a summary of the derivation of the potentials $\phi$ and $\psi$ as obtained by Trubnikov [10]. The quantities that describe the change in the dimensions and shape of a cloud of test particles in a plasma can be found by obtaining the moments for the test particles with respect to the distribution of field particles in velocity space. There are an infinite number of moments, the entire set of which completely describes the distribution of test particles. Taking the time rate of change of these moments provides a complete description of the "spreading" of this cloud of test particles. The time derivatives of the first two moments are

$$\frac{d}{dt} < \Delta v_{ai} > = \frac{d}{dt} \int \Delta v_{ai} f_{\beta}(\vec{v}_\beta') d\vec{v}_\beta' n_\beta$$

$$\frac{d}{dt} < \Delta v_{ai} \Delta v_{aj} > = \frac{d}{dt} \int \Delta v_{ai} \Delta v_{aj} f_{\beta}(\vec{v}_\beta') d\vec{v}_\beta' n_\beta$$

$\alpha$ refers to the test particle scattered by the field particles $\beta$. Subscripts $i$ and $j$ are the indices running through the Cartesian coordinates $x, y$ and $z$. Switching to a center-of-mass reference frame allows one to find the change in the test particle's velocity due to a collision with a field particle. Thus,

$$\vec{v}_\alpha = \vec{R} + \frac{m_\beta}{m_\alpha + m_\beta} \vec{u}$$

where $\vec{u} = \vec{v}_\alpha - \vec{v}_\beta$

from which the change in the test particle's velocity is

$$\Delta \vec{v}_\alpha = \frac{m_\alpha m_\beta}{m_\alpha} \Delta \vec{u}$$

where $\Delta \vec{R} = 0$ since the center of mass velocity remains unaltered. The time derivative is taken at $t = 0$ so that the average velocity at that time equals the initial velocity. The number of particles moving through an infinitesimal cross sectional area $d\sigma = dp d\phi$ is determined from the elementary flux of particles by

$$dn_\beta(\vec{v}_\beta') |d\vec{u}| d\sigma = f_\beta(\vec{v}_\beta') d\vec{v}_\beta' u d\sigma$$
This is multiplied by the components of \( \Delta \vec{v}_\alpha \) and \( \Delta \vec{v}_\alpha \Delta \vec{v}_\alpha \), and integrated over the entire plane whose normal is parallel to the direction of the incident particle prior to being scattered by a fixed center. These are integrated a final time over the elementary fluxes, \( f_\beta (\vec{v}'_\beta) d\vec{v}'_\beta \), to yield

\[
\frac{d}{dt} < \Delta v_{\alpha i} > = \int \left[ \frac{m_\alpha \beta}{m_\alpha} \sum_0^{2\pi} \rho_{\text{max}} \int \Delta u_{i} u \rho d\rho d\phi \right] f_\beta (\vec{v}'_\beta) d\vec{v}'_\beta
\]  

(C.6)

\[
\frac{d}{dt} \Delta v_{\alpha i} \Delta v_{\alpha j} = \int \left[ \left( \frac{m_\alpha \beta}{m_\alpha} \right)^2 \sum_0^{2\pi} \rho_{\text{max}} \int \Delta u_{i} \Delta u_{j} u \rho d\rho d\phi \right] f_\beta (\vec{v}'_\beta) d\vec{v}'_\beta
\]  

(C.7)

\[
\text{If the relative velocity, } \vec{u}, \text{ is taken along the } z\text{-axis then the components of the change in the velocity due to small angle scattering are}
\]

\[
\Delta u_x = u \sin \theta \cos \phi, \quad \Delta u_y = u \sin \theta \sin \phi, \quad \Delta u_z = -u (1 - \cos \theta)
\]  

(C.8)

(see figure 49). The deflected particle’s motion describes a hyperbola and the scattering angle is related to the impact parameter, \( \rho \), by

\[
\tan \frac{\theta}{2} = \frac{\rho_\perp}{\rho}
\]  

(C.9)

\( \rho_\perp \) is the impact parameter obtained from the Rutherford scattering cross section [18] when the particle is deflected through 90° from a Coulomb collision,

\[
\sigma_R (\theta)_{\theta=\pi/2} = \left( \frac{Z_\alpha Z_\beta e^2}{4\pi \varepsilon_0 m_\alpha \beta u^2} \right)^2 \left( \frac{1}{4 \sin^4 \theta/2} \right)_{\theta=\pi/2} = \left( \frac{Z_\alpha Z_\beta e^2}{4\pi \varepsilon_0 m_\alpha \beta u^2} \right)^2 \rho_\perp^2
\]  

(C.10)

One can see that \( \sigma_R (\theta) = 1/u^4 \) and thus \( \rho_\perp = 1/u^2 \). The components of \( \vec{u} \) can be reformulated as
\[ \Delta u_x = 2u \sin \theta \cos \frac{\theta}{2} \cos \varphi = 2u \frac{\rho \rho_1}{\rho^2 + \rho_1^2} \cos \varphi \]
\[ \Delta u_y = 2u \frac{\rho \rho_1}{\rho^2 + \rho_1^2} \sin \varphi, \quad \Delta u_z = -2u \frac{\rho_1^2}{\rho^2 + \rho_1^2} \]

The vector \( w \) has only a \( z \) component since the integration of \( \Delta u_\theta \) and \( \Delta u_\varphi \) over the interval 0 to \( 2\pi \) leads to \( w_x = w_y = 0 \). Therefore,

\[ w_i = \frac{u_i}{u} \frac{m_\alpha}{m} \int_0^{2\pi} \int_0^{\rho_{\text{max}}} \Delta u_i \Delta u_i \rho dp d\varphi \] 

\[ = -\left(1 + \frac{m_\alpha}{m_\beta} \right) \frac{Z_\alpha Z_\beta e^2}{4\pi \varepsilon_0 m_\alpha} \frac{4\pi u_x}{u^2} \int_0^{\rho_{\text{max}}} \frac{\rho dp}{\rho^2 + \rho_1^2} \]

\[ \lambda = \ln \left( \frac{\lambda_\rho}{\rho_1} \right) \]

where the divergent integral has been cutoff at \( \rho_{\text{max}} = \lambda_\rho \), the Debye length, and denoted by \( \lambda \).

The tensor \( w_{ij} \) is diagonal with respect to the velocity components because the integration of \( \Delta u_i \Delta u_i \) over the interval 0 to \( 2\pi \) results in \( w_{ij} = 0 \) when \( i \neq j \). Additionally, \( w_{xx} = w_{yy} \) and \( w_{xx} \ll w_{xy} \) such that \( w_{xy} \) will be taken to equal 0. Therefore,

\[ w_{ij} = \left( \delta_{ij} - \frac{u_i u_j}{u^2} \right) \frac{m_\alpha}{m} \int_0^{\rho_{\text{max}}} \Delta u_i \Delta u_j \rho dp d\varphi \]

\[ = \left( \delta_{ij} - \frac{u_i u_j}{u^2} \right) \frac{Z_\alpha Z_\beta e^2}{4\pi \varepsilon_0 m_\alpha} \frac{4\pi}{u} \int_0^{\rho_{\text{max}}} \frac{\rho^3 dp}{\rho^2 + \rho_1^2} \]

\[ = \lambda - \frac{1}{2} = \lambda \]

Again \( \rho_{\text{max}} = \lambda_\rho \) such that the integral equals \( \lambda \) when \( \lambda \gg 1 \). Let

\[ \Omega = \frac{Z_\alpha^2 Z_\beta^2 e^4}{4\pi \varepsilon_0 m_\alpha} \]

then,
One then has two potential functions that describe the distribution of field particles.

\[ \phi_\beta (\bar{v}_\alpha) = \int [\bar{v}_\alpha - \bar{v}_\beta] f_\beta (\bar{v}_\beta) d\bar{v}_\beta; \]  

(C.19)

\[ \psi_\beta (\bar{v}_\alpha) = \int [\bar{v}_\alpha - \bar{v}_\beta] f_\beta (\bar{v}_\beta) d\bar{v}_\beta \]  

\[ \frac{d}{dt} < \Delta v_{\alpha i} > = \left( 1 + \frac{m_\alpha}{m_\beta} \right) \Omega \int \frac{u_i}{u^3} f_\beta (\bar{v}_\beta) d\bar{v}_\beta \]  

(C.15)

\[ \frac{d}{dt} < \Delta v_{\alpha i} \Delta v_{\alpha j} > = \Omega \int \left( \frac{\delta_{ij}}{u} - \frac{u_i u_j}{u^3} \right) f_\beta (\bar{v}_\beta) d\bar{v}_\beta \]  

(C.16)

\[ \frac{d}{dt} < \Delta v_{\alpha i} > = \left( 1 + \frac{m_\alpha}{m_\beta} \right) \Omega \frac{\partial}{\partial v_{\alpha i}} \int \frac{f_\beta (\bar{v}_\beta)}{|\bar{v}_\alpha - \bar{v}_\beta|} d\bar{v}_\beta \]  

(C.17)

\[ \frac{d}{dt} < \Delta v_{\alpha i} \Delta v_{\alpha j} > = \Omega \frac{\partial^2}{\partial v_{\alpha i} \partial v_{\alpha j}} \int |\bar{v}_\alpha - \bar{v}_\beta| f_\beta (\bar{v}_\beta) d\bar{v}_\beta \]  

(C.18)

These potentials differ from those of Trubnikov by the omission of $-1/(4\pi)$ and $-1/(8\pi)$ from $\phi_\beta$ and $\psi_\beta$, respectively. $\phi_\beta$ is analogous to the potential in electrostatics, the gradient of which produces a field which when multiplied by the effective charge $\Omega \cdot m_\alpha$ generates a force. (C.15) then represents the rate of change of velocity, or acceleration, resulting in the increase or decrease of the test particle's velocity as it moves amongst the field particles. This effect is akin to dynamical friction [19]. $\psi_\beta$ represents the average value of the relative velocity and (C.16) represents the spread of the velocity distribution of the test particles with respect to that of the field particles. The resultant velocity diffusion effect arising from (C.16) would tend to spread the velocity distribution of a group of test particles to match that of the field particles. Furthermore, (C.16) can represent the rate of change in the energy of the cloud of test particles.
Thus,

\[
\frac{d\mathbf{p}_\alpha}{dt} = m_\alpha \frac{d}{dt} <\Delta \mathbf{v}_\alpha > = m_\alpha \left(1 + \frac{m_\alpha}{m_\beta}\right) \Omega \nabla \cdot \phi_\beta (\mathbf{v}_\alpha) \tag{C.20}
\]

\[
\frac{dE_\alpha}{dt} = \frac{m_\alpha}{2} \frac{d}{dt} \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha = m_\alpha \left(\frac{1}{2} <\Delta \mathbf{v}_\alpha \cdot \Delta \mathbf{v}_\alpha > + \mathbf{v}_\alpha \cdot \Delta \mathbf{v}_\alpha \right)
\]

\[
= m_\alpha \Omega \left[\frac{1}{2} \nabla \cdot \phi_\beta (\mathbf{v}_\alpha) + \left(1 + \frac{m_\alpha}{m_\beta}\right) \mathbf{v}_\alpha \nabla \cdot \phi_\beta (\mathbf{v}_\alpha) \right] \tag{C.21}
\]

It is also worth noting that the friction and velocity diffusion arising from (C.15) and (C.16) are velocity dependent, decreasing as \(1/u^2\) due to Coulomb scattering via (C.10).
Appendix D: Implementation of the Drift-Kinetic Model into DIVIMP

The various routines and code modifications that were created to assimilate Reiser's model into DIVIMP as well as the input and output features needed to invoke and display the model will be briefly discussed in this appendix.

D.1 Fortran 77 Routines Developed to Include the Drift-Kinetic Model in DIVIMP

D.1.1 Coulomb Collision Terms

Dirk Reiser provided the Fortran 77 algorithm used to calculate the complete drift and diffusive coefficients (equations 32 a-f in Reiser's paper: 'Improved Kinetic Test Particle Model for Impurity Transport' [6]). Only the terms pertaining to parallel-to-B motion, \( k_1 \) and \( D_{h,5} \), were invoked. The remaining terms were effectively “commented out” to reduce CPU time. Should future considerations wish to investigate impurity motion perpendicular to the field line, \( v_z \), then the full set of drift and diffusive terms can be easily reactivated.

D.1.2 Irreducible Hermite Coefficients

The Hermite coefficients, \( h_{xx}, h_{yy}, \) and \( h_{zz} \) (Appendix A.34 to A.36), are required to evaluate \( K_d \) and \( D_h \). Code was developed to calculate these coefficients based on the average background values of \( Z, n, T, v, \) \( \nabla_T, \) and \( \nabla_v \) for each grid cell. The Hermite coefficients are in turn used to evaluate \( \Lambda \) (A.6), \( \alpha \) (A.16), and \( C_1 \) and \( C_2 \) (A.80).

D.1.3 Background Ion Velocity Gradient

In order to evaluate the Hermite coefficients, the velocity gradient of the background plasma (moving parallel-to-B) needed to be evaluated for each grid cell. Since viscous forces had not been previously considered in DIVIMP, the need for \( \nabla_v \) never arose. Thus a new subroutine has been added.

D.1.4 Linear Interpolation of Background Quantities

Due to the apparent sensitivity of Reiser's thermal gradient force on the background quantities (see section 3.8.2.2), a routine was developed with the help of David Elder to determine the exact values of \( n, T, \) \( T_e, \) and \( v \) between cell centers. This is accomplished by linearly interpolating these values from their averaged values. Stated more precisely, when the ion finds itself at
position 's' between two cell centers on a given ring, the value of say $T_i$ at 's' is calculated from
the slope connecting the average $T_i$ value assigned to the cell center behind the particle to the
average $T_i$ value assigned to the cell center in front of the particle. This would provide a
smoother transition from one cell to the next and eliminate the sudden "jump" in values at the cell
boundaries as occurs when using the average value over the entire cell. (Fortunately, the
combination of FF with FIG reduces the sensitivity experienced by FIG alone such that there is
no significant difference when using either the averaged or the exact background values).

D.1.5 Recalculation of the Hermite Coefficients

Normally, the Hermite coefficients would be calculated based on the average values of the
background quantities for each cell. They would then be stored in an array prior to the initiation
of the main loop incrementing the impurity ion's velocity. This step was done to reduce the
amount of CPU time because instead of having to calculate the coefficients at each time step,
their value would be merely accessed from the array element corresponding to the cell that the ion
happened to be in. Unfortunately, when using the linearly interpolated values, the coefficients
must be evaluated at each time step thereby necessitating the need for a new routine to replace
that of section D.1.2.

D.1.6 Check of the Gradient Scale Lengths

The drift-kinetic model is only valid when the temperature and velocity gradient scale lengths are
larger than the minimum required values as derived in Appendix B. To ensure this, a subroutine
was written to calculate the gradient scale lengths for each grid cell in the SOL and the private
plasma and to compare them to the minimum required values (eqns. (2.12) and (2.13)) as
determined from the values of $T_i$, $n_i$, $v_i$, and $Z_i$ for that cell. When either of the gradient scale
lengths is larger than the minimum value, a warning is written to the screen and the user may
wish to terminate the program. A warning is also written to the .dat file. The values of the
gradient scale lengths for those cells that failed to meet the criteria are written to the .lim file
along with the minimum values. This allows the user to compare the values and adjust the
background quantities $T_i$, $n_i$, and $v_i$ accordingly.

D.1.7 Average Forces and Average Impurity per Grid Cell

In preparation for plotting the results of the drift-kinetic model it was necessary to calculate the
average values per grid cell of the forces and the impurity velocity. FF, FIG, FIV, and the total of
these forces, F_{net}, along with the impurity velocity \( v_z \) are tallied and stored for each grid cell. After all the impurities have been launched and followed, the values are divided by the impurity particle density, \( n_z \), to provide the average forces and velocity for a single ion.

**D.2 Description of the Input Parameters**

**D.2.1 Selection of the Reiser drift-kinetic model**

Activating the drift-kinetic model to increment the impurity ion velocity is achieved in the INPUT data file (having the suffix .d6i) under the listing of

```
  Reiser Coll/Force Option 0=off 1=cell 2=cont  0
```

This input line can be found at the very beginning of the INPUT file just after the Collision option. As observed, the integer value following the character string can take on three values:

0  switches the drift-kinetic model "off" and the parallel transport of impurities is governed by the fluid approximation, eqn. (1.14).

1  switches the drift kinetic model "on" and the coefficients \( \Lambda (A.6) \), \( \alpha (A.16) \), C1 and C2 (A.80) in the drift \( K_4 \) and diffusive \( D_{4z} \) terms are pre-calculated for each grid cell. That is to say, the averaged values of \( n_z, v_z, V_{4z}, T_z \) and \( V_{4} T_{4z} \) assigned to each grid cell in the Main Core, SOL, and Trap regions are used to equate these coefficients once and once only. These values are then stored in arrays, which are drawn upon for each increment of the ion's motion. This was done to reduce the total number of calculations and consequently the CPU time involved.

2  switches the drift kinetic model "on" but this time the \( n_z, v_z, V_{4z}, T_z \) and \( V_{4} T_{4z} \) values used in equating \( \Lambda, \alpha, C1, \) and \( C2 \) are evaluated uniquely for the exact location that the ion happens to occupy within a given cell as discussed in section D.1.4 and D.1.5. The reason for introducing Option 2 is discussed in section 3.8.2.2.

**D.2.2 Selection of the Individual Force Components of the Drift-Kinetic Model**

Selection of the individual components is accomplished according to the following set of INPUT lines:
Master Switch 0off ion -select drift/diffusion: 1

-Drift Coef. K11 f(v-vb, nb) 0off 1on 1
-Drift Coef. K12 f(v-vb, gradTb) 0off 1on 1
-Drift Coef. K13 f(v-vb, gradvb) 0off 1on 1
-Diff. Coef. D11 f(v-vb, nb) 0off 1on 1
-Diff. Coef. D12 f(v-vb, gradTb) 0off 1on 1
-Diff. Coef. D13 f(v-vb, gradvb) 0off 1on 1

The master switch option must be selected as 'on' (i.e. = 1) in order to allow for specific selection/omission of any of the three terms that comprise the drift, \( K_n \), and diffusive, \( D_n \), coefficients. These, in turn, will only be evaluated if the Reiser Collision Option is equal to 1 or 2 (see section D.2.1).

Note: Drift: \( K_t = K11 + K12 + K13 \)

Diffusive: \( D_{tt} = D11 + D12 + D13 \)

Entering a '0' at the end of the line for any of the K and D terms will give it a value of 0. Entering a '1' will evaluate the selected K or D term as expressed in section 2.1 where

\[
K11 = K_d(n_d) \quad (2.4) \quad D11 = D_{tt}(n_d) \quad (2.7)
\]
\[
K12 = K_d(\nabla T_i) \quad (2.5) \quad D12 = D_{tt}(\nabla T_i) \quad (2.8)
\]
\[
K13 = K_d(\nabla v_d) \quad (2.6) \quad D13 = D_{tt}(\nabla v_d) \quad (2.9)
\]

This option was included to allow the user to compare and contrast the behaviour of the drift kinetic model with DIVIMP's fluid approximation model on a term-by-term basis (i.e. comparing the FII's of both models separately from all the other forces).

D.2.3 Combing of the Fluid Approximation with the Drift-kinetic Model:

Combing the two transport models is achieved via the selection:

Fluid Approx. + Drift-kinetic 0off/1on 1

In choosing this option the fluid approximation model replaces the drift-kinetic model whenever the impurity ion enters a region in the SOL or private plasma where either the ion-temperature gradient scale length or the ion-velocity gradient scale length is less than the minimum value required by the drift-kinetic model (see section 2.3).
D.2.4 Selection of Uni-Directional Motion:

Selecting strictly one-way motion of an impurity ion along a magnetic field line is accomplished via:

' Velover. (Terminate Part. Tracking) 0off 1/2on ' 2

0 switches this option 'off' such that the impurity ion will continue to be tracked even when its velocity changes sign.

1 terminates ion tracking the moment its velocity becomes negative.

2 terminates ion tracking the moment its velocity becomes positive.

This option is only useful when observing one ion with no cross-field diffusion. Special care must be exercised in noting the ion's initial direction of motion because no motion will be observed if the ion starts out in the negative direction when Velover = 1. This option also works best when used in conjunction with the individual force selection option (section D.2.2) to generate plots depicting the magnitude and direction of a particular force at various locations along the magnetic field line.

D.3 Description of Plots Generated and their Input Parameters:

The input parameters as they appear in the OUT input file (having suffix .d6o) are presented followed by a brief description.

D.3.1 Poloidal Plots (551-560)

Input Parameters:

$Poloidal Plots of Averaged Forces for a given Charge State.$
$Plots depicted are based upon which ever Ion Transport Model$ was initially selected in the INPUT file:
$Drift-Kinetic Model (as calculated via the Reiser formulation)$
$Fluid Approximation Model (currently employed by DIVIMP)$

'551 Frictional Force iz = 4 ' 1
| '552 | Frictional Force near X pt | iz = 4 | 1 |
| '553 | Thermal Force | iz = 4 | 1 |
| '554 | Thermal Force near X pt | iz = 4 | 1 |
| '555 | Vb-GRAD Force | iz = 4 | 1 |
| '556 | Vb-GRAD Force near X pt | iz = 4 | 1 |
| '557 | Frictional and Thermal Force | iz = 4 | 1 |
| '558 | Fric. and Therm. near X pt | iz = 4 | 1 |
| '559 | Total Force | iz = 4 | 1 |
| '560 | Total Force near X pt | iz = 4 | 1 |

Note: Vb-GRAD force = FIV

Plots 551-560 depict the various forces, which have been averaged over each grid cell. The even numbered plots display these forces near the X-point while the odd numbered plots depict the entire grid. Entering an integer value of 1 after the character string generates a plot and inputting an integer for 'iz' displays the forces acting on the ion of that particular charge state. Scaling and the selection of the number of contour levels are done in exactly the same manner as for other poloidal/contour plots generated in DIVIMP. The reader is thus referred to the Out Reference Manual of DIVIMP for a fuller treatment of these options [7].

D.3.2 Averaged Forces along a Magnetic Flux Tube (575)

Input Parameters:

Note: Ffi = FF, Fth = FIG, and Fvbg = FIV
The emphasis here is on the contributions of the friction and the thermal forces since they tend to dominate. As a result, $F_{\text{net}}$ is then strictly the summation of these forces (along with the FTV contribution when the Reiser option is selected) and the velocity diffusion force. By selecting the three different options of section D.2.1 in turn, one can see the difference in behaviour of the forces when all the other conditions specified in the INPUT file remain unaltered.

**D.3.3 Force Balance Plots of the Drift-Kinetic Model (576,577,578)**

**Input Parameters:**

These plots depict the three forces of the drift-kinetic model corresponding to (2.4), (2.5), and (2.6) for the special case when 1) the impurity ion velocity is 0, 2) the relative velocity between the ion and the background plasma is 0, and 3) the impurity ion velocity is selected by the user (in m/s). It also includes the sum total of these forces, $F_{\text{net}}$. These plots compliment Plot 575 by showing the relative importance of the forces for these special conditions and are useful in identifying potential particle traps in the background plasma. Both the ionization and the ring number must be specified.

**D.3.4 Plots Depicting the Individual Drift Force Components versus CHI (580)**

**Input Parameters:**
Plots showing the individual drift force components and their total:

- Frictional force: FF(DK) and FF(FA)
- Temperature gradient force: FIG(DK) and FIG(FA)
- Velocity gradient force: FIV(DK)
- Net force: Fnet(DK) and Fnet(FA)

Forces are plotted versus CHI

The component forces of the drift-kinetic model corresponding to (2.4), (2.5), and (2.6) along with their total are plotted against chi, χ, ranging from -3 to 3. For comparison, the frictional (1.2) and thermal force (1.4) of the fluid approximation is also plotted along with their total. The plot relates the magnitudes and directions of the forces to each other under various user-defined conditions and is thus a very useful tool in demonstrating how each component contributes to the overall force acting on the particle. The user has the option to observe the behaviour of these forces when χ⊥ is set equal to χ∥. Selecting the integer 1 in the input line just under the designation Xper does this. Selecting χ⊥ to be 0 restricts the behaviour to be solely along the B-field line. The selection of the physical properties is achieved by inputting values under the corresponding headings that appear in the input line 580. These values are entered on the line 000 and must be entered in the same order as they appear on line 580. It does not matter if the values in line 000 fall exactly under the headings of line 578 so long as the order of the entries is preserved.

Note:

- Zb = Background ionization integer
- Z = Impurity ionization integer
- mb = Background ion mass (a.m.u.) integer
- m = Impurity ion mass (a.m.u.) integer
- nb = Background density (m⁻³) real
- Tbg = Background temperature gradient (eV/m) real
\( T_b \) = Background temperature (eV) \\
\( v_{bg} \) = Background velocity gradient (1/s)

**D.3.5 Plots Depicting the Individual Diffusive Terms versus CHI (581)**

**Input Parameters:**

- Plots showing the individual diffusive components and their total:
- Drift-kinetic: \( D(n_b) + D(T_{bg}) + D(v_{bg}) = D_{net(DK)} \)
- Fluid Approximation: \( D(FA) \)
- Diffusive terms are plotted versus CHI

```
'581  Zb, Z, mb, m, nb, Tbg, Tb, vbg, Xper' 1
'000' 1 2 2 12 5e18 3.0 20.0 3e4 1
'581  Zb, Z, mb, m, nb, Tbg, Tb, vbg, Xper' 0
'000' 1 4 2 12 6e18 2.5 90.0 0.0 0
```

The terms involved in the velocity diffusion force of the drift-kinetic model, (2.7), (2.8), and (2.9), along with their total are plotted against CHI, \( \chi \), ranging from -3 to 3. For comparison, the term from the pressure gradient force of the fluid approximation,

\[
D(FA) = \frac{2kT_z}{m_z} \frac{1}{\tau_{||}}
\]

(4.1))

is also plotted. Again the same specifications are employed as for Plot 580.

Note: \( D(n_b) = D_{tk}(n_i) \), \( D(T_{bg}) = D_{tk}(\nabla T) \), \( D(v_{bg}) = D_{tk}(\nabla v) \), \( D(FA) = D_{IFA} \) and \( D_{net(DK)} = D_{tk}D_{net(DK)} \)

**D.3.6 Plot of 1/C \_1 versus CHI (582)**

**Input Parameters:**

- Plot of the inverse of \( C_1(+) \) and \( C_1(-) \) versus CHI to determine the limits of \( C_1 \) for which the drift-kinetic model remains valid.
Evaluation of Cl used in FIG(DK)  

$\frac{1}{C_1^+}$ and $\frac{1}{C_1^-}$, as defined in Appendix B, are plotted versus CHI (where $\chi = \xi d$). Each pair of $\frac{1}{C_1^+}$ and $\frac{1}{C_1^-}$ values corresponds to negative and positive values of $\chi$. The region between a given pair of plotted values represents those values of $\frac{1}{C_1^+}$ and $\frac{1}{C_1^-}$ for which the drift-kinetic model is invalid with regard to the effect of the ion temperature gradient.

D.3.7 Plot of $\frac{1}{C_1}$ versus CHI (583)

Input Parameters:

1. Plot of the inverse of $C_2(\pm)$ versus CHI to determine the limits of $C_2$ for which the drift-kinetic model remains valid.

Evaluation of $C_2$ used in FIG(DK)  

$\frac{1}{C_2^+}$ and $\frac{1}{C_2^-}$, as defined in Appendix B, are plotted versus CHI (where $\chi = \xi d$). Each pair of $\frac{1}{C_2^+}$ and $\frac{1}{C_2^-}$ values corresponds to negative and positive values of $\chi$. The region between a given pair of plotted values represents those values of $\frac{1}{C_2^+}$ and $\frac{1}{C_2^-}$ for which the drift-kinetic model is invalid with regard to the effect of the ion velocity gradient.

D.3.8 Averaged Ion Velocity along a Magnetic Flux Tube (585)

Input Parameters:

1. Averaged Ion Velocity Plots along the Field Line for a given Ring and Charge State. Plots depicted are based upon which ever Ion Transport Model was initially selected in the INPUT file:
   - Drift-Kinetic Model (as calculated via the Reiser formulation)
   - Fluid Approximation Model (currently employed by DIVIMP)
The velocity of the impurity ion as averaged over the grid cells is depicted along the length of a particular magnetic field line, or ring. Both the ionization and ring number must be specified. The averaged values of $\alpha$ and $\chi_{\alpha}$ are also plotted. These have been calculated using the averaged velocity values in conjunction with the cell-averaged values of $T_i$ and $v_i$ as determined from the selections made in the INPUT file.