A model for plasma-neutral fluid interaction and its application to a study of CT formation in a magnetised Marshall gun

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Abstract

A model for plasma/neutral fluid interaction was developed and included in the DELiTE code framework implementation of non-linear MHD equations. The source rates of ion, electron and neutral fluid momentum and energy due to ionization and recombination were derived using a simple method that enables determination of the volumetric rate of thermal energy transfer from electrons to photons and neutral particles in the radiative recombination reaction. This quantity cannot be evaluated with the standard formal procedure of taking moments of the relevant collision operator, and has been neglected in other studies. The plasma/neutral fluid interaction model was applied to study CT formation in the SPECTOR magnetised Marshall gun, enabling clarification of the mechanisms behind the significant increases in CT electron density that are routinely observed well after formation. Neutral gas, which remains concentrated below the gas valves after CT formation, diffuses up the gun barrel to the CT containment region where it is ionized, leading to the observed electron density increases. This understanding helps account for the exceptionally significant increase in temperature, and markedly reduced density, observed during the electrode edge biasing experiment conducted on SPECTOR. It is thought that edge fueling impeditment, a consequence of a biasing-induced transport barrier, is largely responsible for the observed temperature increase and density decrease.

1 Introduction

The DELiTE (Differential Equations on Linear Triangular Elements) framework [1, 2] was developed for spatial discretisation of partial differential equations on an unstructured triangular grid in axisymmetric geometry. The framework is based on discrete differential operators in matrix form, which are derived using linear finite elements and mimic some of the properties of their continuous counterparts. A single-fluid two-temperature MHD code with anisotropic thermal diffusion was implemented in this framework. The inherent properties of the operators are used in the code to ensure global conservation of energy, particle count, toroidal flux, and angular momentum. As described in [1, 2, 3], the code was applied to study a novel experiment in which a compact torus (CT), produced with the SMRT (Super Magnetized Ring Test) magnetised Marshall gun, is magnetically levitated off an insulating wall and then magnetically compressed through the action of currents in the levitation/compression coils located outside the wall. The code also has the capability to start magnetic compression from a Grad-Shafranov equilibrium. There are simulated diagnostics for magnetic probes, interferometers, ion-Doppler measurements, and CT $q$ profile. Special care was taken to simulate the poloidal vacuum field in the insulating region between the inner radius of the insulating wall and the levitation/compression coils, and to couple this solution to the MHD solutions in the plasma domain, while maintaining toroidal flux conservation, enabling a quantitative model of plasma/wall interaction in various coil configurations.

The initial motivation for including plasma/neutral fluid interaction in the MHD model was to reduce simulated ion temperature to levels corresponding to the ion-Doppler diagnostic measurements while maintaining system energy conservation, i.e., while keeping $\nu_{num} = \nu_{phys}$, where $\nu_{num}$ [m$^2$/s] is the (isotropic) viscosity diffusion coefficient that is used in the viscous stress tensor in the momentum equation, and $\nu_{phys}$ [m$^2$/s] is used in the viscous stress tensor in the ion energy equation. While a certain minimum level of viscosity diffusion (velocity field smoothing) is required for numerical stability, it is possible to reduce simulated ion...
temperature by setting $\nu_{\text{phys}} < \nu_{\text{num}}$, but this breaks the energy conservation property of the numerical scheme. In practice, for formation simulations with a mesh of practical resolution ($h_0 \sim 2\text{mm}$), it is found that we need to use a value of $\nu_{\text{num}} \geq 400 \text{ m}^2/\text{s}$ to maintain sufficiently smooth velocity fields. Charge exchange collisions are an important mechanism by which ion temperature is reduced - in a charge exchange reaction, a hot ion takes an electron from a cold neutral particle, resulting in a hot neutral particle and a cold ion. Secondly, it was expected that the presence of a neutral fluid in the gun around the gas valves, which is also a physical phenomenon, would slow down the axially directed plasma during the CT formation process, leading to reduced viscous heating. In the actual experiment, as described in [1, 2, 3], the CT formation process is initiated when an electric field is applied across a cloud of cold gas between the inner and outer machine electrodes. The gas cloud is concentrated near the gas-puff valves. The gas valves are typically opened approximately 400$\mu$s before the formation voltage is applied across the electrodes, so that a neutral gas cloud has ample time to diffuse away from the valves. The ionization action of the applied formation field results in seed electrons that lead to further impact ionization. The resultant plasma that is advected up the gun by the $\mathbf{J} \times \mathbf{B}_0$ force is initially surrounded by a relatively static neutral gas cloud that it ionizes or displaces. The neutral cloud slows down the advected plasma through collisions, resulting in a reduction of ion viscous heating as $\mathbf{v}$ and $\nabla \mathbf{v}$ are reduced. It turns out that, while the inclusion of a neutral fluid in the CT formation simulations did reduce simulated ion temperature, the cause of the temperature reduction was due to bulk inertial effects, which reduce axial velocities and therefore reduces viscous heating, rather than direct interaction between the fluids. It was found that the same level of ion temperature reduction can be achieved in simulations without a neutral fluid, simply by increasing the initial plasma fluid density until it is equal to the combined neutral fluid and plasma densities for a simulation with the same initial spatial distributions of the neutral and plasma fluids. Furthermore, due to equilibration between the ion and electron temperatures, ionization rates are high in regions where ions are hot, so that neutral fluid density, and hence the level of charge-exchange related ion cooling, is approximately negligible in those key regions.

Electron impact ionization, and radiative recombination are inelastic reactive collisions, whereas the resonant charge exchange process is an elastic reactive collision because the initial and final states are degenerate. The procedure, described in [4, 5], of taking moments of the charge exchange collision operator, cannot be avoided when evaluating the terms in the plasma fluid and neutral fluid momentum and energy corresponding to charge exchange reactions. However, to derive the terms in the fluid equations corresponding to ionization and recombination, instead of taking moments of the corresponding collision operators, as done in [4, 5], a more straightforward and intuitive method is used. We directly evaluate the effect of the particle sources and sinks arising from to ionization and recombination on the species (ion, electron, neutral) momentums and energies (note that charge exchange reactions do not lead to particle sources or sinks). This approach also allows for determination of the terms that must be included in the MHD equations when external particle sources are present. The strategy has the additional benefit that it allows for the evaluation of $Q_{e\rightarrow i}^\text{rec}$, the thermal energy transferred from electrons to neutral particles due to recombination per volume per second. By contrast, the moment-taking method used in [4, 5], allows for the evaluation of $Q_{i\rightarrow e}^\text{rec}$(rate of thermal energy transferred from ions to neutral particles due to recombination), but leads to an entangled integral expression for $Q_{e\rightarrow i}^\text{rec}$ that can’t be easily evaluated, so that $Q_{i\rightarrow e}^\text{rec}$ is retained while the $Q_{e\rightarrow i}^\text{rec}$ term is neglected from the species energy equations.

The model for plasma / neutral fluid interaction proved to be useful because it helped clarify the mechanisms behind the significant increases in electron density that are routinely observed at $\sim 500\mu$s after CT formation in the SPECTOR (Spherical Compact Toroid) plasma injector at General Fusion Inc. [6] (note that this was not observed with the SMRT injector [1, 2, 3], as CTs produced in that configuration lasted for less than 500$\mu$s). In the SPECTOR plasma injector, neutral gas, which remains concentrated below the gas valves after CT formation, diffuses up the gun barrel to the CT containment region where it is ionized, leading to the observed electron density increases. This understanding helps account for the exceptionally significant increase in temperature, and markedly reduced density, observed during the electrode edge biasing experiment conducted on SPECTOR [7]. It is thought that edge fueling impediment, a consequence of a biasing-induced transport barrier, is largely responsible for the observed temperature increase and density decrease.

This paper is arranged as follows. An overview of the model for plasma-neutral fluid interaction is presented in section 2. Development of the scattering terms, and the reactive terms pertaining to ionization, recombination and charge exchange collisions, that are included in the plasma and neutral fluid equations,
is presented in sections 3 and 4 respectively. The resultant fluid equations for ions, electrons and neutral particles are derived in section 5. The ion and electron MHD equations are reduced to a set of single plasma fluid equations, that include terms pertaining to interaction with the neutral fluid, in section 6. A demonstration of total system energy and particle count conservation with inclusion of a neutral fluid in the MHD model is presented and discussed in section 7. Results pertaining to neutral fluid interaction, from simulations of CT formation, levitation and magnetic compression [1, 2, 3] in the SMRT plasma injector, and from simulations of CT formation in the SPECTOR plasma injector [6], are presented and discussed in section 8. Section 9 concludes the paper with an overview of the principal findings.

2 Model overview

Based on the work presented in [4, 5], the model includes resonant charge exchange, electron impact ionization, and radiative recombination reactions:

\[ \begin{align*}
    i^+ + n &\rightarrow n + i^+ \\
    e^- + n &\rightarrow i^+ + 2e^- - \phi_{\text{ion}} \\
    e^- + i^+ &\rightarrow n + h\nu_p
\end{align*} \]

(2.1)

Here, \( i^+ \), \( e^- \) and \( n \) respectively represent singly charged ions and electrons, and neutral particles, \( h \, [m^2 \text{kg/s}] \) is Planck’s constant, and \( \nu_p \) is the wave frequency associated with the photon emitted in the recombination reaction. The charge exchange process is resonant because the initial and final states have the same quantum mechanical energy - the exchanged electron’s initial and final energy states are the same so that the combined kinetic energy and momentum of the ion and neutral is unchanged [8, 9]. In the following derivations, singly charged ions and a single neutral species will be considered. The plasma is assumed to be optically thin, so that radiation energy \( h\nu_p \) associated with radiative recombination is lost from the system. Following from [4, 5], excited states are not tracked in order to simplify the model. Instead, an effective ionization potential, \( \phi_{\text{ion}} \), includes the excitation energy that is expended on average for each ionization event, as well as the electron binding energy.

The Boltzmann equation for species \( \alpha \) is

\[ \frac{\partial f_\alpha}{\partial t} + \nabla \cdot (V f_\alpha) + \nabla_v \cdot \left( \frac{q_\alpha}{m_\alpha} (E(r,t) + V \times B(r,t)) \right) f_\alpha = \frac{\partial f_\alpha}{\partial t} |_{\text{collisions}} = C_\alpha(f) \]

where \( \alpha = i, e, \text{ or } n \) denote ions, electrons, or neutral particles. If \( \alpha = n \), then the acceleration term vanishes, because \( q_n = 0 \). The collision operator can be split into parts pertaining to elastic scattering collisions and reacting collisions: \( C_\alpha(f) = C^{\text{scatt.}}_\alpha(f) + C^{\text{react.}}_\alpha(f) \).

3 Scattering collision terms

Mass, momentum and energy are conserved and particles are not created or destroyed in elastic scattering collisions. The Coulomb interaction of charged particles is a long range one characterised by multiple simultaneous interactions. The short range fields (within the electronic shells) of neutral particles result, by contrast, in binary collisions. Because of the long range nature of the Coulomb force, small-angle deflections associated with Coulomb collisions are much more frequent than the large angle deflections associated with binary collisions. The cumulative effect of many small-angle collisions is much larger than that of relatively fewer large-angle collisions [8]. It is possible to deal with multiple collisions by approximating them as a number of simultaneous binary collisions [10]. Boltzmann’s collision operator for neutral gas is :

\[ C^{\text{scatt.}}_\alpha(f) = \sum_{\sigma} C^{\text{scatt.}}_{\alpha\sigma}(f_\alpha, f_\sigma) \]

(3.1)

Here, \( C^{\text{scatt.}}_{\alpha\sigma}(f_\alpha, f_\sigma) \), the rate of change of \( f_\alpha \) due to collisions of species \( \alpha \) with species \( \sigma \), considers only binary collisions and is therefore bilinear because \( C^{\text{scatt.}}_{\alpha\sigma} \) is a linear function of both its arguments [11, 9]. In plasmas, where long-range Coulomb interactions lead to Debye shielding, a many-body effect, collisions
are not strictly binary. However, in a weakly coupled plasma, the departure from bilinearity is logarithmic, and can be neglected to a good approximation since the logarithm is a relatively weakly varying function [12]. The collisional process for the elastic collisions described by $C^{scatt.}$ conserves particles, momentum and energy at each point [9].

Particle conservation is expressed by:

$$\int C^{scatt.}_{\alpha\sigma} d\mathbf{V} = 0$$  \hspace{1cm} (3.2)

In combination with equation 3.1, this yields

$$\int C^{scatt.}_{\alpha} d\mathbf{V} = 0$$  \hspace{1cm} (3.3)

i.e., scattering collisions have no $0^{th}$ moment effect. To find the contribution of scattering collisions to the rates of change of momentum of the ions, electrons and neutral particles, the first moments of the operators for scattering collisions can be taken. The total friction force (collisional momentum exchange) acting on species $\alpha$ due to the net effect of the frictional interaction with each of species $\sigma$ is defined as:

$$\mathbf{R}_\alpha = \Sigma_{\sigma} \mathbf{R}_{\alpha\sigma} = \int m_\alpha \Sigma_{\sigma} C^{scatt.}_{\alpha\sigma} \mathbf{V} d\mathbf{V} = \int m_\alpha C^{scatt.}_{\alpha} \mathbf{V} d\mathbf{V}$$  \hspace{1cm} (3.4)

Here, $\mathbf{R}_{\alpha\sigma}$ is the frictional force exerted by species $\sigma$ on species $\alpha$. We define

$$c_\alpha(\mathbf{r},t) = \mathbf{V} - \mathbf{v}_\alpha(\mathbf{r},t)$$  \hspace{1cm} (3.5)

as the species random velocity relative to $\mathbf{v}_\alpha$, the species fluid velocity [10]. Then, because the statistical average of a random quantity is zero, and, since the average of an averaged value is unchanged, we have:

$$\int \mathbf{v}_\alpha f_\alpha d\mathbf{V} = \mathbf{v}_\alpha$$  \hspace{1cm} (3.6)

Note that, using equations 3.5, 3.6, 3.3, and 3.4, we can write: $\mathbf{R}_\alpha = \int m_\alpha C^{scatt.}_{\alpha} c_\alpha d\mathbf{V}$. In a system with just two species, ions and electrons, $\mathbf{R}_\alpha$ is given by the Chapman-Enskog closures:

$$\mathbf{R}_e = -\mathbf{R}_i = \eta' ne \mathbf{J} - 0.71n \nabla T_e$$  \hspace{1cm} (3.7)

Ignoring the thermal force for simplicity, this is: $\mathbf{R}_e = -\mathbf{R}_i = \eta' ne \mathbf{J} = \nu e \rho_e (\mathbf{v}_i - \mathbf{v}_e)$. When there are just two species, then, since $\mathbf{R}_\alpha = \Sigma_{\sigma} \mathbf{R}_{\alpha\sigma}$ (equation 3.4) and $\mathbf{R}_{\sigma\sigma} = 0$ (a fluid does not exert friction on itself), the equivalent notation $\mathbf{R}_e \equiv R_{ei}$ and $\mathbf{R}_i \equiv R_{ie}$ can be introduced for the frictional forces due to scattering collisions.

The notation $(X)_{scatt.}$ is introduced to represent the part of $X$ that pertains to scattering collisions. The first moment of the first term of the Boltzmann equation is $\frac{\partial (\mathbf{v}_\alpha m_\alpha n_\alpha)}{\partial t}$. Since

$$\left( \frac{\partial (\mathbf{v}_\alpha m_\alpha n_\alpha)}{\partial t} \right)_{scatt.} = \rho_\alpha \left( \frac{\partial \mathbf{v}_\alpha}{\partial t} \right)_{scatt.} + \mathbf{v}_\alpha \left( \frac{\partial \rho_\alpha}{\partial t} \right)_{scatt.},$$

and scattering collisions are not a source of particles

$$\Rightarrow \left( \frac{\partial \rho_\alpha}{\partial t} \right)_{scatt.} = 0,$$

the terms $\rho_\alpha \left( \frac{\partial \mathbf{v}_\alpha}{\partial t} \right)_{scatt.}$ can be expressed as:

$$\rho_\alpha \left( \frac{\partial \mathbf{v}_\alpha}{\partial t} \right)_{scatt.} = \mathbf{R}_\alpha = \Sigma_{\sigma} \mathbf{R}_{\alpha\sigma}$$  \hspace{1cm} (3.8)

With the inclusion of a neutral fluid, for the individual species, this is:

$$\rho_i \left( \frac{\partial \mathbf{v}_i}{\partial t} \right)_{scatt.} = \mathbf{R}_i = \mathbf{R}_{ie} + \mathbf{R}_{in}$$

$$\rho_e \left( \frac{\partial \mathbf{v}_e}{\partial t} \right)_{scatt.} = \mathbf{R}_e = \mathbf{R}_{ei} + \mathbf{R}_{en} = -\mathbf{R}_{ie} + \mathbf{R}_{en}$$  \hspace{1cm} (3.9)

$$\rho_n \left( \frac{\partial \mathbf{v}_n}{\partial t} \right)_{scatt.} = \mathbf{R}_n = \mathbf{R}_{ni} + \mathbf{R}_{ne} = -\mathbf{R}_{en} - \mathbf{R}_{en}$$
where the identities $\mathbf{R}_{\alpha\sigma} = -\mathbf{R}_{\sigma\alpha}$ (implying that the frictional force exerted by species $\alpha$ on species $\sigma$ is balanced by the frictional force exerted by species $\sigma$ on species $\alpha$) have been used. Just as $\mathbf{R}_{ei} = \nu_{ei} \rho_e (\mathbf{v}_e - \mathbf{v}_i)$ and $\mathbf{R}_{iem} = \nu_{iem} \rho_m (\mathbf{v}_m - \mathbf{v}_i)$, the forms for the charged-neutral friction forces are $\mathbf{R}_{in} = \nu_{in} \rho_i (\mathbf{v}_n - \mathbf{v}_i)$ and $\mathbf{R}_{en} = \nu_{en} \rho_e (\mathbf{v}_n - \mathbf{v}_e)$, where $\nu_{\sigma \alpha} \sim \frac{m_\sigma}{m_\alpha} \nu_{\alpha \sigma}$ is the frequency for scattering of particles of species $\sigma$ from particles of species $\alpha$ [11]. The terms $\mathbf{R}_{im}$ and $\mathbf{R}_{en}$ can be neglected in many cases - in general, neutral-charged particle scattering collisions are unimportant when the plasma is ionized by even a few percent [8, 4].

To find the contribution of scattering collisions to the rates of change of energy of the ions, electrons and neutral particles, the second moments of the operators for scattering collisions can be taken. Collisional energy conservation requires that $Q_{L\alpha\sigma} + Q_{L\sigma\alpha} = 0$, where

$$Q_{L\alpha\sigma} = \int C_{\alpha\sigma}^{scatt.} \left( \frac{1}{2} m_\alpha V^2 \right) dV$$

is the rate at which species $\sigma$ collision ally transfers energy to species $\alpha$. The $L$ subscript is to indicate that the kinetic energy of both species is measured in the same (e.g. Laboratory) frame. $Q_{\alpha\sigma} = \int C_{\alpha\sigma}^{scatt.} \left( \frac{1}{2} m_\alpha v^2 \right) dV$ is the rate at which species $\sigma$ collision ally transfers energy to species $\alpha$ in the rest frame of species $\alpha$ (the frame moving at $v_\alpha$, the fluid velocity of species $\alpha$) [12, 9]. The total rate of collisional energy transfer to species $\alpha$ in the rest frame of species $\alpha$ is

$$Q_\alpha = \sum_\sigma Q_{\alpha\sigma}$$

(3.11)

Using equation 3.5 in equation 3.10, it can be shown that

$$Q_{L\alpha\sigma} = \int C_{\alpha\sigma}^{scatt.} \left( \frac{1}{2} m_\alpha (c_\alpha + v_\alpha)^2 \right) dV = Q_{\alpha\sigma} + v_\alpha \cdot \mathbf{R}_{\alpha\sigma}$$

so that:

$$\sum_\sigma Q_{L\alpha\sigma} = \int C_{\alpha\sigma}^{scatt.} \left( \frac{1}{2} m_\alpha V^2 \right) dV = Q_\alpha + v_\alpha \cdot \mathbf{R}_\alpha$$

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\[
\frac{1}{\gamma - 1} \left( \frac{\partial p_i}{\partial t} \right)_{\text{scatt.}} = Q_{ie} + Q_{in}
\]
\[
\frac{1}{\gamma - 1} \left( \frac{\partial p_e}{\partial t} \right)_{\text{scatt.}} = Q_{ei} + Q_{en}
\]
\[
\frac{1}{\gamma - 1} \left( \frac{\partial p_n}{\partial t} \right)_{\text{scatt.}} = Q_{ni} + Q_{ne}
\]

Here, \( Q_{\alpha \sigma} \) represents the heat gained by species \( \alpha \) due to scattering interaction with species \( \sigma \). Again, due to the relative unimportance of neutral-charged particle scattering collisions \([8, 4]\), the terms \( Q_{in}, Q_{en}, Q_{ni}, \) and \( Q_{ne} \) can usually be neglected.

4 Reactive collision terms

In this section, the terms in the species (ions, electrons and neutral fluids) mass, momentum and energy conservation equations that pertain to collisions associated with ionization, recombination, and charge exchange reactions will be assessed.

4.1 Ionization and recombination

4.1.1 Mass Conservation

As shown in \([4, 5]\), the sources and sinks in the species continuity equations that arise from ionization and recombination reactions can be evaluated by taking the zeroth moments of the collision operators pertaining to ionization and recombination collisions. Alternatively, a more intuitive method that doesn’t use the collision operators is presented in \([8]\). The mean free path for impact ionization collisions is defined by considering that there is one particle in the volume swept out by the cross-sectional area for impact ionization collisions over one mean free path:

\[
n_n \sigma_{\text{ion}} (V_{\text{rel}}) \frac{1}{\lambda_{\text{ion}} mfp} = 1.
\]

Here, \( V_{\text{rel}} = |V_e - V_n| \), the relative particle speed for the ionization reaction, where \( V_e \) is the electron particle velocity and \( V_n \) is the neutral particle velocity. Since \( m_n \gg m_e \), \( V_{\text{rel}} \approx V_e \). The frequency for electron impact ionization collisions is defined as an average over all velocities in the Maxwellian distribution:

\[
\nu_{\text{ion}} = \frac{V_{\text{rel}}}{\lambda_{\text{ion}} mfp} \approx n_n <\sigma_{\text{ion}} V_e >
\]

From this, \( \Gamma_{\text{ion}}^i \), the rate of increase of ions per unit volume due to ionization reactions is

\[
\Gamma_{\text{ion}}^i = \Gamma_{\text{ion}}^e = -\Gamma_{\text{n}}^i = n_n n_e <\sigma_{\text{ion}} V_e >
\]

Here, \( \Gamma_{\text{ion}}^e \) and \( \Gamma_{\text{ion}}^i \) are the rates of increase of electrons and neutral particles per unit volume due to ionization reactions. The velocity-space-integrated quantity \( <\sigma_{\text{ion}} V_e > [\text{m}^3/\text{s}] \) is the ionization rate parameter; its value can be found as a function of temperature from the fitting formula given by Voronov \([13]\), as

\[
<\sigma_{\text{ion}} V_e > (r, t) = A \left( 1 + P \sqrt{U} \right) \frac{U^K exp (-U)}{U + X}
\]

where \( U(r, t) = \frac{\phi_{\text{ion}}}{T_e(r, t)} \), with \( \phi_{\text{ion}} \) being the effective ionization potential in the same units as \( T_e \). Following from \([4, 5]\), an effective ionization potential including the excitation energy that is expended on average for each ionization event, as well as the electron binding energy, is used instead of the regular ionization energy, because, for simplicity, excited states are not tracked. An estimate of the validity of the formula for the ionization rate parameter is given by Voronov for each element. For example, for hydrogen, accuracy is to within 5% for electron temperatures from 1 eV to 20 keV. The DELiTE MHD code has the option of either hydrogen, deuterium or helium as the neutral gas and plasma source. From \([13]\), the coefficients required
for equation 4.1 for these options are shown in table 1. Also included is the atomic diameter ($d_{\text{atom}}$) for each atom, which is used to calculate the viscous and thermal diffusion coefficients for the neutral fluid. The values for effective ionization potentials are taken from [14].

| ion type : | H   | D   | He  |
|-----------|-----|-----|-----|
| $\phi_{\text{ion}}$[eV]  | 13.6| 33  | 28  |
| $A$       | $2.91 \times 10^{-14}$[m$^3$/s] | $2.91 \times 10^{-14}$[m$^3$/s] | $1.75 \times 10^{-14}$[m$^3$/s] |
| $P$       | 0   | 0   | 0   |
| $K$       | 0.39| 0.39| 0.35|
| $X$       | 0.232| 0.232| 0.18|
| $d_{\text{atom}}$[m]  | $1.06 \times 10^{-10}$ | $2.4 \times 10^{-10}$ | $2.8 \times 10^{-10}$ |

Table 1: Coefficients for calculating ionization rate parameters

The rate of increase of ions per unit volume due to recombination reactions can be evaluated by considering the mean free path and collision frequency associated with recombination [8] as

$$\Gamma_i^{\text{rec}} = \Gamma_e^{\text{rec}} = -\Gamma_n^{\text{rec}} = \int C_e^{\text{rec}} dV = -n_e n_i < \sigma_{\text{rec}} V_e >$$  

The velocity integrated quantity $< \sigma_{\text{rec}} V_e >$ [m$^3$/s] is the recombination rate parameter - its value for recombination to charge state $Z_{\text{eff}} - 1$ can be estimated as a function of electron temperature as [15, 5, 8]

$$< \sigma_{\text{rec}} V_e > (r, t) = 2.6 \times 10^{-19} \frac{Z_{\text{eff}}^2}{\sqrt{T_e(r, t)[eV]}}$$  

Hence, the mass continuity equations for the three-fluid system are:

$$\dot{n}_i = -\nabla \cdot (n_i v_i) + \Gamma_i^{\text{ion}} - \Gamma_i^{\text{rec}}$$

$$\dot{n}_e = -\nabla \cdot (n_e v_e) + \Gamma_e^{\text{ion}} - \Gamma_e^{\text{rec}}$$

$$\dot{n}_n = -\nabla \cdot (n_n v_n) + \Gamma_n^{\text{rec}} - \Gamma_n^{\text{ion}} + \Gamma_n^{\text{ext}}$$  

Note that all source terms here, as well as each of $n_\alpha$ and $v_\alpha$, are functions of $r$ and $t$. In the magnetic compression experiment [2, 3], the plasma injector gas puff valves take time to shut, and remain open for several hundred microseconds after the formation banks are fired, so neutral particles are being added to the system near the valves. An additional neutral external source term, $\Gamma_n^{\text{ext}}(r, t)$ [m$^{-3}$ s$^{-1}$], has been included on the right side of the expression for $\dot{n}_n$, in order to be able to this simulate neutral particle injection.

4.1.2 Momentum Conservation

As shown in [4, 5], the sources and sinks in the species momentum equations that arise from ionization and recombination reactions can be evaluated by taking the first moments of the relevant collision operators. Here, the formal process of taking first moments (and second moments for the contributions to the rates of change of energy) is skipped, to arrive at results equivalent to those presented in [4, 5], but with evaluation of the $Q^{\text{rec}}$ term.

Referring to equation 4.4, the general form of the expression for the species rates of change of number density that correspond to the reactive collisions of ionization and recombination, and also to any external particle sources, is

$$\frac{\partial n_\alpha}{\partial t} = \sum_k S_{ak}$$  

Here, $(X)_{\text{ire}}$ denotes the part of $X$ that pertains to the reactive collisions of ionization and recombination, and to any external particle sources. $S_{ak}$ [m$^{-3}$s$^{-1}$] represents the $k^{\text{th}}$ source (in units of particles per metres cubed per second) for particles of type $\alpha$, as determined from equation 4.4. Here, $S_{i1} = S_{e1} = -S_{n2} =$
Each neutral particle introduced by recombination initially has momentum \(\rho_\alpha v_\alpha\). Meanwhile, ions with velocity \(v_i\) and \(v_e\) contribute to the total ion momentum, and newly ionized particles are introduced with velocity \(m_i v_i + m_e v_e\). The corresponding additional terms on the right side of the momentum equations are:

\[
\frac{\partial (\rho_\alpha n_\alpha v_\alpha)}{\partial t} = -\nabla \cdot \mathbf{P}_\alpha - \nabla \cdot (\rho_\alpha n_\alpha v_\alpha) + g_\alpha n_\alpha (E + v_\alpha \times \mathbf{B}) + \mathbf{R}_\alpha
\]

To include the terms that correspond to the reactive collisions of ionization and recombination, and to any external particle sources, this can be written as:

\[
\frac{\partial (m_\alpha n_\alpha v_\alpha)}{\partial t} = \ldots + \left( \frac{\partial (m_\alpha n_\alpha v_\alpha)}{\partial t} \right)_{irce},
\]

where \(\ldots\) represents the right side of equation 4.6. Particles sourced by \(S_{ak}\) add, or (for sources with negative sign), remove, species \(m_\alpha n_\alpha v_\alpha\) momentum, where \(m_\alpha\) and \(v_\alpha\) are the mass and initial fluid velocity of the particles of type \(j\) which have their momentum introduced or taken away. The summation over sources of type \(j\) is relevant only for \(S_{ak} = S_{n1} = \Gamma_{rec}\), recombination is a source for total neutral particle momentum, and each neutral particle added to the neutral population through recombination initially has momentum \(m_i v_i + m_e v_e\). The general form of the expression for the species rates of change of momentum that correspond to the reactive collisions of ionization and recombination, and also to any external particle sources, is:

\[
\left( \frac{\partial (m_\alpha n_\alpha v_\alpha)}{\partial t} \right)_{irce} = \sum_k \left( S_{ak} \sum_j (m_{0jk} v_{0jk}) \right)
\]

This expression must be retained for the neutral recombination source term \(S_{n1}\). However, for all other source terms, \(\sum_j (m_{0jk} v_{0jk}) \rightarrow m_\alpha n_\alpha v_\alpha\), where \(v_0\) is the "initial" fluid velocity (i.e., the fluid velocity at the time when the ionization or recombination reaction occurs) of the particles of type \(\alpha\) which are introduced or taken away due to source \(S_{ak}\), and the general expression can be simplified to:

\[
\left( \frac{\partial (m_\alpha n_\alpha v_\alpha)}{\partial t} \right)_{irce} = m_\alpha \sum_k (S_{ak} v_{0k})
\]

The corresponding additional terms on the right side of the momentum equations are:

\[
\frac{\partial (m_i n_i v_i)}{\partial t} = \Gamma_{i}^{\text{ion}} m_i v_i - \Gamma_{n}^{\text{rec}} m_i v_i
\]

\[
\frac{\partial (m_e n_e v_e)}{\partial t} = \Gamma_{i}^{\text{ion}} m_e v_e - \Gamma_{n}^{\text{rec}} m_e v_e
\]

\[
\frac{\partial (m_n n_n v_n)}{\partial t} = \Gamma_{n}^{\text{rec}} (m_i v_i + m_e v_e) - \Gamma_{i}^{\text{ion}} m_n v_n + \Gamma_{n}^{\text{ext}} m_n v_{n0}
\]

For example, in the expression above for \(\left( \frac{\partial (m_i n_i v_i)}{\partial t} \right)_{irce}\), ions that are sourced from neutral particles through ionization add to the total ion momentum, and newly ionized particles are introduced with velocity \(v_i\). Meanwhile, ions with velocity \(v_i\), that are lost to recombination, take away from the total ion momentum. Each neutral particle introduced by recombination initially has momentum \(m_i v_i + m_e v_e\). Neutral particles introduced by external sources such as gas puffing also add neutral particle momentum - each externally sourced neutral has initial momentum \(m_n v_{n0}\), where \(v_{n0}\) is its initial velocity.

Using equation 4.5, equation 4.7 can be recast as:

\[
\left( \frac{\partial (m_\alpha n_\alpha v_\alpha)}{\partial t} \right)_{irce} = m_\alpha n_\alpha \left( \frac{\partial v_\alpha}{\partial t} \right)_{irce} + m_\alpha v_\alpha \left( \frac{\partial m_\alpha}{\partial t} \right)_{irce} = \sum_k \left( S_{ak} \sum_j (m_{0jk} v_{0jk}) \right)
\]

\[
\Rightarrow m_\alpha n_\alpha \left( \frac{\partial v_\alpha}{\partial t} \right)_{irce} = \sum_k \left( S_{ak} \sum_j (m_{0jk} v_{0jk}) \right) - m_\alpha v_\alpha \left( \sum_k S_{ak} \right)
\]

(4.9)
For the ions and electrons (all sources), and for the neutral source terms corresponding to ionization and external sources, where \( \sum_j (m_{0jk}v_{0jk}) \rightarrow m_\alpha v_k \), this general expression can be simplified to

\[
m_\alpha n_\alpha \left( \frac{\partial v_\alpha}{\partial t} \right)_{ire} = m_\alpha \sum_k (S_{\alpha k} (v_{0k} - v_\alpha))
\]

(4.10)

Equation 4.10 and (for neutral recombination only) equation 4.9 lead to:

\[
\begin{align*}
\rho_i \left( \frac{\partial v_i}{\partial t} \right)_{ire} &= \Gamma_{i^{\text{ion}}} n_i (v_n - v_i) \\
\rho_e \left( \frac{\partial v_e}{\partial t} \right)_{ire} &= \Gamma_{i^{\text{ion}}} n_e (v_n - v_e) \\
\rho_n \left( \frac{\partial v_n}{\partial t} \right)_{ire} &= \Gamma_{\text{rec}} (m_i v_i + m_e v_e - m_\alpha v_n) + \Gamma_{\text{ext}} m_\alpha (v_{n0} - v_n)
\end{align*}
\]

(4.11)

### 4.1.3 Energy Conservation

Assuming Maxwellian distributions for each of species \( \alpha \), so that \( p_\alpha = n_\alpha T_\alpha \), the part of the species energy equation that corresponds to particle sources due to the reactive collisions of ionization and recombination, and to external particle sources, can be written as

\[
\left( \frac{\partial}{\partial t} \left( \frac{1}{2} m_\alpha n_\alpha v_\alpha^2 + \frac{p_\alpha}{\gamma - 1} \right) \right)_{ire} = \frac{1}{2} \sum_j \left( S_{\alpha k} \sum_j (m_{0jk} v_{0jk}^2) \right) + \frac{1}{\gamma - 1} \sum_k \left( \xi_{\alpha k} S_{\alpha k} \Sigma T_{0jk} \right)
\]

(4.12)

Here, \( \xi_{\alpha k} \) is a particle mass ratio that must be considered for the ionization source that introduces ions \( (S_{1i} = \Gamma_{i^{\text{ion}}}^i) \) and electrons \( (S_{1e} = \Gamma_{i^{\text{ion}}}^e) \), and for the recombination source that introduces neutral particles \( (S_{1n} = \Gamma_{\text{rec}}^n) \). To clarify this for the ionization source, when a neutral particle with thermal energy \( \frac{1}{\gamma - 1} T_n \) is ionized, the resultant ion and electron have thermal energies \( \frac{m_i}{m_\alpha} \frac{1}{\gamma - 1} T_n \) and \( \frac{m_e}{m_\alpha} \frac{1}{\gamma - 1} T_n \) respectively, so that their combined thermal energy is equal to that of the original neutral.

To clarify the relevance of \( \xi_{\alpha k} \) for the recombination source, simple analysis of the kinematics of the radiative recombination reaction indicates that the bulk of the electron thermal energy, and a fraction of the ion thermal energy, is transferred to the emitted photon. Noting that \( m_i \sim m_n \gg m_e \), then, in the rest frame of the neutral particle (post reaction), the ion (prior to the reaction) has negligible kinetic energy (i.e., thermal energy, since we are considering single particles with random velocities), the electron has approximately the same energy that it has in the laboratory frame, and the neutral particle has no kinetic energy. Consequently, as an approximation, the bulk of the electron thermal energy (of the order \( (m_e/m_n) T_e/(\gamma - 1) \)) and a negligible portion of the ion thermal energy (\( \sim (m_i/m_n) T_i/(\gamma - 1) \)) is transferred to the photon emitted in the radiative recombination reaction, while a negligible portion of the electron thermal energy (of the order \( \sim (m_e/m_n) T_e/(\gamma - 1) \)) and the bulk of the ion thermal energy (\( \sim (m_i/m_n) T_i/(\gamma - 1) \)) is transferred to the neutral particle. The combined thermal energy of the neutral particle and photon is equal to the combined thermal energy of the ion and electron. Note that for \( \Gamma_{\text{ext}} \), the external neutral particle source, \( \xi_{\alpha k} = 1 \).

Once again, the summation over \( j \) is relevant only for \( S_{\alpha k} = S_{n1} = \Gamma_{\text{rec}} \); recombination is a source for neutral particle energy, and it is assumed that each neutral particle added to the neutral particle population through recombination initially has energy \( \frac{1}{2} (m_i v_i^2 + m_e v_e^2) + \frac{1}{\gamma - 1} \left( \frac{m_i}{m_\alpha} T_i + \frac{m_e}{m_\alpha} T_e \right) \). Note that for all other sources (apart from recombination) the summation over \( j \) in equation 4.12 can be neglected; \( \Sigma T_{0jk} \rightarrow T_{0k} \), where \( T_{0k} \) is the initial temperature of the sourced particle, and \( \sum_j (m_{0jk} v_{0jk}^2) \rightarrow m_\alpha v_{0k}^2 \). We want to obtain an expression for \( \left( \frac{\partial p_\alpha}{\partial t} \right)_{ire} \), which will be included on the right side of the species energy equations which have the form

\[
\frac{1}{2} m_\alpha v_\alpha^2 \left( \frac{\partial p_\alpha}{\partial t} \right)_{ire} + m_\alpha n_\alpha v_\alpha \cdot \left( \frac{\partial v_\alpha}{\partial t} \right)_{ire} + \frac{1}{\gamma - 1} \left( \frac{\partial p_\alpha}{\partial t} \right)_{ire} = \frac{1}{2} \sum_j \left( S_{\alpha k} \sum_j (m_{0jk} v_{0jk}^2) \right) + \frac{1}{\gamma - 1} \sum_k \left( \xi_{\alpha k} S_{\alpha k} \Sigma T_{0jk} \right)
\]

\[
\Rightarrow \frac{1}{\gamma - 1} \left( \frac{\partial p_\alpha}{\partial t} \right)_{ire} = \frac{1}{\gamma - 1} \sum_k \left( \xi_{\alpha k} S_{\alpha k} \Sigma T_{0jk} \right) + \frac{1}{\gamma - 1} \sum_k \left( S_{\alpha k} \sum_j (m_{0jk} v_{0jk}^2) \right) - \frac{1}{2} m_\alpha v_\alpha^2 \sum_k (S_{\alpha k} - m_\alpha n_\alpha v_\alpha \cdot \left( \frac{\partial v_\alpha}{\partial t} \right)_{ire})
\]
Using equation 4.9, this implies that

\[
\left( \frac{\partial p_{\alpha}}{\partial t} \right)_{ire} = \sum_k \left( \xi_{ak} S_{ak} \Sigma j \tau_{ojk} \right) + (\gamma - 1) \left[ \frac{1}{2} \sum_k \left( \frac{\partial}{\partial t} \left( S_{ak} \Sigma j \left( m_{ojk} v_{ojk}^2 \right) \right) \right) \right] - \frac{1}{2} m_{\alpha} v_{\alpha}^2 \sum_k (S_{ak}) - v_{\alpha} \cdot \left( \sum_k \left( S_{ak} \Sigma j \left( m_{ojk} v_{ojk} \right) \right) - m_{\alpha} v_{\alpha} \left( \Sigma S_{ak} \right) \right)
\]

\Rightarrow \left( \frac{\partial p_{\alpha}}{\partial t} \right)_{ire} = \sum_k \left( \xi_{ak} S_{ak} \Sigma j \tau_{ojk} \right) + (\gamma - 1) \left[ \frac{1}{2} m_{\alpha} v_{\alpha}^2 \sum_k (S_{ak}) + \sum_k \left( S_{ak} \Sigma j \left( m_{ojk} \left( \frac{1}{2} v_{ojk}^2 - v_{\alpha} \cdot v_{ojk} \right) \right) \right) \right]

\Rightarrow \left( \frac{\partial p_{\alpha}}{\partial t} \right)_{ire} = \sum_k \left( \xi_{ak} S_{ak} \Sigma j \tau_{ojk} \right) + (\gamma - 1) \left( \sum_k \left( S_{ak} \left( \frac{1}{2} m_{\alpha} v_{\alpha}^2 + \sum_j \left( m_{ojk} \left( \frac{1}{2} v_{ojk}^2 - v_{\alpha} \cdot v_{ojk} \right) \right) \right) \right) \right)

(4.13)

For the ions and electrons (all sources), and for the neutral source terms corresponding to ionization and external sources, where \( \sum m_{ojk} v_{ojk} \rightarrow m_{\alpha} v_{0k} \), \( \sum \left( m_{ojk} v_{ojk}^2 \right) \rightarrow m_{\alpha} v_{0k}^2 \), and \( \sum \tau_{ojk} \rightarrow \tau_{0k} \), this general expression can be simplified to

\[
\left( \frac{\partial p_{\alpha}}{\partial t} \right)_{ire} = \sum_k \left( \xi_{ak} S_{ak} \tau_{0k} \right) + (\gamma - 1) \left( \frac{1}{2} m_{\alpha} \sum_k \left( S_{ak} \left( \frac{1}{2} v_{\alpha}^2 + 2 v_{\alpha} \cdot v_{0k} + v_{0k}^2 \right) \right) \right)
\]

\Rightarrow \left( \frac{\partial p_{\alpha}}{\partial t} \right)_{ire} = \sum_k \left( \xi_{ak} S_{ak} \tau_{0k} \right) + (\gamma - 1) \left( \frac{1}{2} m_{\alpha} \sum_k \left( S_{ak} \left( v_{\alpha} - v_{0k} \right)^2 \right) \right)

However, the more complicated form of equation 4.13 must be retained for the recombination neutral source term.

The resultant forms for the individual species are:

\[
\left( \frac{\partial p_{i}}{\partial t} \right)_{ire} = \Gamma_{i}^{ion} \frac{m_{i}}{m_{n}} T_{n} - \Gamma_{i}^{rec} \tau_{i} + (\gamma - 1) \frac{1}{2} m_{i} \left( \Gamma_{i}^{ion} \left( \mathbf{v}_{i} - \mathbf{v}_{n} \right) \right)^2
\]

\[
\left( \frac{\partial p_{n}}{\partial t} \right)_{ire} = \Gamma_{n}^{ion} \frac{m_{n}}{m_{i}} T_{i} - \Gamma_{n}^{rec} T_{e} + (\gamma - 1) \left( \Gamma_{i}^{ion} \frac{1}{2} m_{e} \left( \mathbf{v}_{e} - \mathbf{v}_{n} \right)^2 - \phi_{ion} \right)
\]

\[
\left( \frac{\partial p_{e}}{\partial t} \right)_{ire} = \Gamma_{e}^{rec} \frac{m_{i}}{m_{n}} T_{i} + \frac{m_{e}}{m_{n}} T_{e} - \Gamma_{i}^{ion} T_{n} + \Gamma_{ext} T_{n0} + (\gamma - 1) \left( \Gamma_{n}^{rec} \frac{1}{2} m_{n} v_{n}^2 + \frac{1}{2} m_{i} v_{i}^2 \right)
\]

\[
+ \frac{1}{2} m_{e} v_{e}^2 - m_{i} v_{i} \cdot \mathbf{v}_{i} - m_{e} v_{e} \cdot \mathbf{v}_{e} \right) + \Gamma_{ext} \frac{1}{2} m_{n} \left( \mathbf{v}_{n} - \mathbf{v}_{n0} \right)^2 \right)
\]

(4.14)

Here, \( T_{n0} \) is the initial temperature of the externally sourced neutral particles. The effective ionization energy has been included as a sink of electron energy - recalling that \( U_{Th} = \frac{P}{\gamma - 1} \), for each electron with energy \( \frac{1}{2} m_{e} \left( \frac{m_{e}}{m_{n}} T_{n} + \frac{1}{2} m_{e} \left( \mathbf{v}_{e} - \mathbf{v}_{n} \right)^2 \right) \) Joules that is sourced by ionization, another electron has expended \( \phi_{ion} \) Joules to initiate the ionization process.

The following definitions are made, representing the thermal energy per unit volume per second transferred between species due to ionization and recombination processes:

\[
Q_{n}^{ion} = \Gamma_{i}^{ion} \frac{1}{\gamma - 1} T_{n} \quad \text{(neutral particles → ions and electrons, due to ionization)}
\]

\[
Q_{i}^{rec} = \Gamma_{n}^{rec} \frac{1}{\gamma - 1} T_{i} \quad \text{(ions → neutral particles (and photons), due to recombination)}
\]

\[
Q_{e}^{rec} = \Gamma_{n}^{rec} \frac{1}{\gamma - 1} T_{e} \quad \text{(electrons → photons (and neutral particles), due to recombination)}
\]

(4.15)
Hence, equation 4.14 can be re-expressed as:

\[
\frac{\partial n_i}{\partial t}_{ire} = (\gamma - 1) \left( \frac{m_i}{m_n} Q_{n}^{ion} - Q_{i}^{rec} + \frac{1}{2} m_i \left( \Gamma_{i}^{ion} (v_i - v_n)^2 \right) \right)
\]

\[
\frac{\partial n_e}{\partial t}_{ire} = (\gamma - 1) \left( \frac{m_e}{m_n} Q_{n}^{ion} - Q_{e}^{rec} + \Gamma_{i}^{ion} \left( \frac{1}{2} m_e (v_e - v_n)^2 - \phi_{ion} \right) \right)
\]

\[
\frac{\partial n_m}{\partial t}_{ire} = (\gamma - 1) \left[ \frac{m_i}{m_n} Q_{i}^{rec} + \frac{m_e}{m_n} Q_{e}^{rec} - Q_{n}^{ion} \right]
\]

\[
+ \Gamma_{n}^{rec} \left( \frac{1}{2} m_n v_n^2 + \frac{1}{2} m_i v_i^2 + \frac{1}{2} m_e v_e^2 - m_i v_n \cdot v_i - m_e v_n \cdot v_e \right)
\]

\[
+ \Gamma_{n}^{ext} \frac{1}{2} m_n (v_n - v_{n0})^2 \right)\]  

(4.16)

In the derivations presented in [4, 5], $Q_{e}^{rec}$ (thermal energy transferred from electrons to neutral particles due to recombination, per m$^3$ per second) is not evaluated because its derivation with the moment-taking method leads to an integral that cannot be evaluated. It is suggested that this term can be dropped if the loss of electron thermal energy due to recombination is not expected to play an important role in the energy balance [4, 5]. However, from equation 4.15, it can be seen that $Q_{e}^{rec} \sim T_i$, so that in cases where $T_i \sim T_e$, it would be unreasonable to neglect $Q_{e}^{rec}$ while retaining $Q_{i}^{rec}$.

The $Q_{e}^{rec}$ term is included as an undetermined energy sink/source for the electron/neutral fluids respectively in [4, 5], without scaling by the factor $m_e/m_n$ in the neutral fluid energy equation, and is ignored when the equations are implemented to code. When implemented to the DELiTE framework MHD code, it was found that inclusion of the $Q_{e}^{rec}$ term as an energy source for the neutral fluid (without the scaling factor $m_e/m_n$ in equation 4.16) leads to significant increases in neutral particle temperature, as shown in section 8.1.

However, as discussed above, from looking at the kinematics of the radiative recombination reaction, it is more physical to neglect $Q_{e}^{rec}$ as an energy source for the neutral fluid, but include it as an energy sink for the electron fluid, while $Q_{i}^{rec}$ may be included as both an energy source for the neutral fluid and an energy sink for the ion fluid. As discussed in section 8.1, peak electron temperature falls by around just one percent when the $Q_{e}^{rec}$ term is included as energy sink for the electron fluid. Overall, in the regimes studied, it turns out that the $Q_{e}^{rec}$ term can be neglected without significantly affecting electron temperature.

### 4.2 Charge exchange

In order to find the terms in the MHD equations that correspond to the charge exchange reactions, the process of taking moments of the charge exchange collision operators can’t be avoided due to, and is complicated by, the degeneracy associated with the charge exchange reaction. In this work, the details of the process won’t be reproduced - only the required results that were originally achieved in [16], and then very well detailed in [4, 5], will be presented.

Taking the zeroth moment of the moment of the charge exchange collision operator leads to the source rate of neutral particles, equal to the source rate of ions, for the charge exchange reaction:

\[
\Gamma_{cx} = n_i n_n \sigma_{cx} (V_{cx}) v_{cx}
\]  

(4.17)

Note $\sigma_{cx}$[m$^2$], the cross section for charge exchange reactions, is evaluated at $V_{cx}$, where $V_{cx}$ is a representative speed for charge exchange collisions [16, 4]:

\[
V_{cx} = \sqrt{\frac{4}{\pi} V_{hi}^2 + \frac{4}{\pi} V_{thn}^2 + v_{in}^2}
\]  

(4.18)

where $V_{thi}$ and $V_{thn}$ are the thermal speeds of the ions and neutral particles, and $v_{in} = |v_{in}| = |v_i - v_n|$. A formula for $\sigma_{cx}(V_{cx})$[m$^2$] can be found based on charge exchange data from Barnett [17, 5]. For hydrogen
and deuterium the fitting formulae are
\[
\sigma_{ex-H}(V_{ex}) = 1.12 \times 10^{-18} - 7.15 \times 10^{-20} \ln(V_{ex})
\]
\[
\sigma_{ex-D}(V_{ex}) = 1.09 \times 10^{-18} - 7.15 \times 10^{-20} \ln(V_{ex})
\]  
(4.19)

Taking the first moment of the charge exchange collision operator leads to
\[
\rho_i \left( \frac{\partial v_i}{\partial t} \right)_{ex} \approx -m_i v_{in} \Gamma_{ex}^{ci} - R_{ni}^{ce} + R_{in}^{ce}
\]
\[
\rho_n \left( \frac{\partial v_n}{\partial t} \right)_{ex} \approx m_i v_{in} \Gamma_{ex}^{ni} + R_{ni}^{ce} - R_{in}^{ce}
\]  
(4.20)

where the notation \((X)_{ex}\) is introduced here to represent the part of \(X\) that pertains to charge exchange collisions, in the same way that \((X)_{ire}\) is the part of \(X\) relating to ionization, recombination and external sources, the term \(m_i v_{in} \Gamma_{ex}^{ci}\) represents the transfer of momentum due to bulk fluid effects \([4, 5]\), and \(R_{ni}^{ce}\) and \(R_{in}^{ce}\) represent frictional drag forces that arise due to charge exchange:

\[
R_{in}^{ce} \approx -m_i \sigma_{ex}(V_{ex}) n_i n_n v_{in} V_{thn}^2 \left( 4 \left( \frac{4}{\pi} \frac{V_{thi}^2 + v_{in}^2}{V_{thn}^2} \right) + \frac{9\pi}{4} \frac{V_{thi}^2}{V_{thn}^2} \right)^{-\frac{1}{2}}
\]
\[
R_{ni}^{ce} \approx m_i \sigma_{ex}(V_{ex}) n_i n_n v_{in} V_{thi}^2 \left( 4 \left( \frac{4}{\pi} \frac{V_{thi}^2 + v_{in}^2}{V_{thn}^2} \right) + \frac{9\pi}{4} \frac{V_{thi}^2}{V_{thn}^2} \right)^{-\frac{1}{2}}
\]  
(4.21)

Such frictional terms do not arise for the ionization and recombination processes, in which the electron thermal speed is assumed to be far higher than the relative particle motion \([4, 5]\). The derivation of the moments of the reacting collision operators assumes that the reacting species are described by Maxwellian distributions. As a result, non-Maxwellian effects due to thermal gradients are neglected and don’t appear in the expressions for \(R_{ni}^{ce}\) and \(R_{in}^{ce}\) \([4]\), as they did in the expressions for \(R_{xi}\) and \(R_{ix}\) (equation 3.7).

Taking the second moment of the charge exchange collision operator leads to
\[
\left( \frac{\partial P}{\partial t} \right)_{ex} \approx (\gamma - 1) \left( \Gamma_{ex}^{ci} \frac{1}{2} m_i v_{in}^2 - v_{in} \cdot R_{in}^{ce} + Q_{in}^{ex} - Q_{ni}^{ex} \right)
\]
\[
\left( \frac{\partial P_n}{\partial t} \right)_{ex} \approx (\gamma - 1) \left( \Gamma_{ex}^{ni} \frac{1}{2} m_i v_{in}^2 + v_{in} \cdot R_{ni}^{ce} - Q_{in}^{ex} + Q_{ni}^{ex} \right)
\]  
(4.22)

where \(Q_{in}^{ce}\) and \(Q_{ni}^{ex}\) represent the transfer of thermal energy \([4, 5]\) associated with charge exchange reactions:

\[
Q_{in}^{ce} \approx m_i \sigma_{ex}(V_{ex}) n_i n_n \frac{3}{4} V_{thn}^2 \sqrt{\frac{4}{\pi} \frac{V_{thi}^2 + 64}{9\pi} \frac{V_{thi}^2}{V_{thn}^2} + v_{in}^2}
\]
\[
Q_{ni}^{ce} \approx m_i \sigma_{ex}(V_{ex}) n_i n_n \frac{3}{4} V_{thi}^2 \sqrt{\frac{4}{\pi} \frac{V_{thi}^2 + 64}{9\pi} \frac{V_{thi}^2}{V_{thn}^2} + v_{in}^2}
\]  
(4.23)

Note that the term \(-v_{in} \cdot R_{ex}^{ce}\) in the ion energy equation represents the rate of frictional work done by neutral fluid on the ion fluid as a result of charge exchange reactions, and the similar term \(v_{in} \cdot R_{ex}^{ce}\) in the neutral fluid energy equation represents the rate of frictional work done by \(R_{ex}^{ce}\), which acts on the neutral fluid with relative velocity \(v_{in}\).

5 3-fluid MHD equations

\((X)_{CE}, (X)_{scatt}, (X)_{react}, (X)_{ext}, (X)_{ire}, \) and \((X)_{ex}\) are, respectively, the parts of \(X\) that pertain to the combination of collisions and external sources, to scattering collisions, to reacting collisions, to external sources, to the combination of ionization, recombination and external sources, and to charge exchange collisions. These quantities are related as
\[
(X)_{CE} = (X)_{scatt} + (X)_{react} + (X)_{ext} = (X)_{scatt} + (X)_{ire} + (X)_{ex}
\]
Combining equations 3.9, 4.11, and 4.20, and using the identity \( \mathbf{v}_{\text{in}} = \mathbf{v}_i - \mathbf{v}_n \), the complete set of terms that arise in the species momentum equations due to scattering and reactive collisions, and an external neutral particle source can be assembled:

\[
\left( \frac{\partial \mathbf{v}_i}{\partial t} \right)_{\text{CE}} = \frac{1}{\rho_i} \left( \mathbf{R}_{\text{ie}} + \mathbf{R}_{\text{in}} - \Gamma_i^{\text{ion}} m_i \mathbf{v}_{\text{in}} - \Gamma_i^{\text{ex}} m_i \mathbf{v}_{\text{in}} - \mathbf{R}_{\text{ni}}^{\text{ex}} + \mathbf{R}_{\text{in}}^{\text{ex}} \right) \\
\left( \frac{\partial \mathbf{v}_e}{\partial t} \right)_{\text{CE}} = \frac{1}{\rho_e} \left( \mathbf{R}_{\text{ei}} + \mathbf{R}_{\text{en}} + \Gamma_i^{\text{ion}} m_e (\mathbf{v}_n - \mathbf{v}_e) \right) \\
\left( \frac{\partial \mathbf{v}_n}{\partial t} \right)_{\text{CE}} = \frac{1}{\rho_n} \left( \mathbf{R}_{\text{ni}} + \mathbf{R}_{\text{ne}} + \Gamma_n^{\text{rec}} (m_i \mathbf{v}_i + m_e \mathbf{v}_e - m_n \mathbf{v}_n) \\
+ \Gamma_n^{\text{ex}} m_n (\mathbf{v}_{\text{in}0} - \mathbf{v}_n) + \Gamma_n^{\text{ex}} m_i \mathbf{v}_{\text{in}} + \mathbf{R}_{\text{ni}}^{\text{ex}} - \mathbf{R}_{\text{in}}^{\text{ex}} \right)
\]

Similarly, combining equations 3.15, 4.16, and 4.22, the equivalent set of terms in the species energy equations are:

\[
\left( \frac{\partial \rho_i}{\partial t} \right)_{\text{CE}} = (\gamma - 1) \left[ Q_{\text{ie}} + Q_{\text{in}} + \frac{m_i}{m_n} Q_i^{\text{ion}} - Q_i^{\text{rec}} + \frac{1}{2} m_i (\Gamma_i^{\text{ion}} + \Gamma_i^{\text{ex}}) v_i^2 \\
- \mathbf{v}_{\text{in}} \cdot \mathbf{R}_{\text{ei}}^{\text{ex}} + Q_{\text{in}}^{\text{ex}} - Q_{\text{ni}}^{\text{ex}} \right] \\
\left( \frac{\partial \rho_e}{\partial t} \right)_{\text{CE}} = (\gamma - 1) \left( Q_{\text{ei}} + Q_{\text{en}} + \frac{m_e}{m_n} Q_e^{\text{ion}} - Q_e^{\text{rec}} + \Gamma_i^{\text{ion}} \left( \frac{1}{2} m_e (\mathbf{v}_e - \mathbf{v}_n)^2 - \phi_{\text{ion}} \right) \right) \\
\left( \frac{\partial \rho_n}{\partial t} \right)_{\text{CE}} = (\gamma - 1) \left[ Q_{\text{ni}} + Q_{\text{ne}} + \frac{m_i}{m_n} Q_i^{\text{rec}} + \frac{m_e}{m_n} Q_e^{\text{rec}} - Q_n^{\text{ion}} + Q_n^{\text{rec}} \left( \frac{1}{2} m_n v_n^2 + \frac{1}{2} m_i v_i^2 + \frac{1}{2} m_e v_e^2 - m_i \mathbf{v}_n \cdot \mathbf{v}_i \\
- m_e \mathbf{v}_n \cdot \mathbf{v}_e \right) + \Gamma_n^{\text{ex}} m_n (\mathbf{v}_{\text{in}0} - \mathbf{v}_n)^2 + \Gamma_n^{\text{ex}} \frac{1}{2} m_i v_i^2 + \mathbf{v}_{\text{in}} \cdot \mathbf{R}_{\text{ni}}^{\text{ex}} - Q_{\text{in}}^{\text{ex}} + Q_{\text{ni}}^{\text{ex}} \right] + \Gamma_n^{\text{ex}} T_{\text{in}0}
\]

5.1 Mass conservation

Mass conservation is expressed by equation 4.4:

\[
\dot{n}_i = -\nabla \cdot (n_i \mathbf{v}_i) + \Gamma_i^{\text{ion}} - \Gamma_i^{\text{rec}} \\
\dot{n}_e = -\nabla \cdot (n_e \mathbf{v}_e) + \Gamma_i^{\text{ion}} - \Gamma_i^{\text{rec}} \\
\dot{n}_n = -\nabla \cdot (n_n \mathbf{v}_n) + \Gamma_n^{\text{rec}} + \Gamma_n^{\text{ex}}
\]

5.2 Momentum conservation

The expression for species momentum conservation in the two-fluid system (ions and electrons, equation 4.6) can be re-expressed as:

\[
\frac{\partial \mathbf{v}_\alpha}{\partial t} = - (\mathbf{v}_\alpha \cdot \nabla) \mathbf{v}_\alpha + \frac{1}{\rho_\alpha} \left( -\nabla p_\alpha - \nabla \cdot \mathbf{f}_\alpha + g_\alpha n_\alpha (\mathbf{E} + \mathbf{v}_\alpha \times \mathbf{B}) + \mathbf{R}_\alpha \right)
\]

This can be combined with equation 5.1 for the species momentum equations in the three-fluid system. The term \( \frac{1}{\rho_n} \mathbf{R}_n \), which arose by taking the first moment of the collision operator for scattering collisions only, is
replaced with the terms in equation 5.1 to yield:

\[
\frac{\partial \mathbf{v}_i}{\partial t} = -\mathbf{v}_i \cdot \nabla p_i - \gamma p_i \mathbf{v}_i + (\gamma - 1) \left[ -\nabla \mathbf{p}_i - \nabla \cdot \mathbf{\pi}_i + q_i n_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B}) + \mathbf{R}_{ie} + \mathbf{R}_{in} \right] \\
- \Gamma_{i}^{\text{ion}} m_i \mathbf{v}_{in} - \Gamma_{i}^{\text{ex}} m_i \mathbf{v}_{in} - \mathbf{R}^{\text{ex}}_{i} + \mathbf{R}^{\text{ex}}_{in}
\]

\[
\frac{\partial \mathbf{v}_e}{\partial t} = -\mathbf{v}_e \cdot \nabla p_e - \gamma p_e \mathbf{v}_e + (\gamma - 1) \left[ -\nabla \mathbf{p}_e - \nabla \cdot \mathbf{\pi}_e + q_e n_e (\mathbf{E} + \mathbf{v}_e \times \mathbf{B}) + \mathbf{R}_{ei} + \mathbf{R}_{en} \right] \\
+ \Gamma_{i}^{\text{ion}} m_e (\mathbf{v}_n - \mathbf{v}_e)
\]

\[
\frac{\partial \mathbf{v}_n}{\partial t} = -\mathbf{v}_n \cdot \nabla p_n - \gamma p_n \mathbf{v}_n + (\gamma - 1) \left[ -\nabla \mathbf{p}_n - \nabla \cdot \mathbf{\pi}_n + \mathbf{R}_{ni} + \mathbf{R}_{ne} + \Gamma_{n}^{\text{rec}} (m_i \mathbf{v}_i + m_e \mathbf{v}_e - m_n \mathbf{v}_n) \right] \\
+ \Gamma_{e}^{\text{ex}} m_i \mathbf{v}_{in} + \mathbf{R}^{\text{ex}}_{ni} - \mathbf{R}^{\text{ex}}_{in} + \Gamma_{n}^{\text{ext}} m_n (\mathbf{v}_{n0} - \mathbf{v}_n)
\]

(5.4)

5.3 Energy conservation

The expression for species energy conservation in the two-fluid system (ions and electrons) is:

\[
\frac{\partial \rho \alpha}{\partial t} = -\mathbf{v}_\alpha \cdot \nabla \rho \alpha - \gamma \rho \alpha \mathbf{v}_\alpha + (\gamma - 1) \left[ -\nabla \mathbf{p}_\alpha - \nabla \cdot \mathbf{\Pi}_\alpha + Q_{\alpha} + Q_{\alpha n} \right]
\]

This can be combined with equation 5.2 for the species energy equations in the three-fluid system. The term 

\((\gamma - 1) Q_{\alpha}, \) which arose by taking the second moment of the collision operator for scattering collisions only, is replaced with the terms in equation 5.2. The resultant species energy equations for the three-fluid system are:

\[
\frac{\partial \rho_i}{\partial t} = -\mathbf{v}_i \cdot \nabla p_i - \gamma p_i \mathbf{v}_i + (\gamma - 1) \left[ -\nabla \mathbf{p}_i - \nabla \cdot \mathbf{q}_i + Q_{ie} + Q_{in} \right] \\
- Q_i^{\text{rec}} + \frac{1}{2} m_i (\Gamma_{i}^{\text{ion}} + \Gamma_{i}^{\text{ex}}) v_{in}^2 - \nabla \mathbf{v}_i \cdot \mathbf{R}^{\text{ex}}_{in} + \mathbf{Q}^{\text{ex}}_{in} - Q_{ni}
\]

\[
\frac{\partial \rho_e}{\partial t} = -\mathbf{v}_e \cdot \nabla p_e - \gamma p_e \mathbf{v}_e + (\gamma - 1) \left[ -\nabla \mathbf{p}_e - \nabla \cdot \mathbf{q}_e + Q_{ei} + Q_{en} \right] \\
+ \frac{m_e}{m_n} Q_{e}^{\text{ion}} - Q_{e}^{\text{rec}} + \Gamma \left[ \frac{1}{2} m_e (\mathbf{v}_e - \mathbf{v}_n)^2 - \phi_{i}^{\text{ion}} \right]
\]

\[
\frac{\partial \rho_n}{\partial t} = -\mathbf{v}_n \cdot \nabla p_n - \gamma p_n \mathbf{v}_n + (\gamma - 1) \left[ -\nabla \mathbf{p}_n - \nabla \cdot \mathbf{q}_n + Q_{ni} + Q_{ne} \right] \\
+ \frac{m_i}{m_n} Q_{i}^{\text{rec}} + \frac{m_e}{m_n} Q_{e}^{\text{rec}} \left[ \frac{1}{2} m_i v_{in}^2 + \frac{1}{2} m_i v_{n}^2 + \frac{1}{2} m_e v_{e}^2 - m_i \mathbf{v}_n \cdot \mathbf{v}_i - m_e \mathbf{v}_n \cdot \mathbf{v}_e \right] + \Gamma^{\text{ex}} \frac{1}{2} m_i v_{in}^2 \\
+ \nabla \mathbf{v}_n \cdot \mathbf{R}^{\text{ex}}_{ni} + \mathbf{Q}^{\text{ex}}_{in} + \Gamma^{\text{ext}} \frac{1}{2} m_n (\mathbf{v}_n - \mathbf{v}_{n0})^2 + \Gamma^{\text{ext}} T_{n0}
\]

6 2-fluid MHD equations

Using standard methods for the terms in the 3-fluid MHD equations that don’t correspond to interspecies collisions, and summing terms corresponding to interspecies collisions, with the limit \(m_e \to 0,\) the ion and electron conservation equations can be reduced to a single plasma-fluid description. In the limit \(m_e \to 0,\) the single plasma-fluid velocity is approximately the ion fluid velocity as is clarified by the identities \(\mathbf{v} = \frac{1}{\rho} \sum \rho_\alpha \mathbf{v}_\alpha\) and \(\rho = \sum \rho_\alpha,\) so that \(\mathbf{v}_{in} \to (\mathbf{v} - \mathbf{v}_n).\) The charged-neutral particle frictional forces \(\mathbf{R}_{in} = -\mathbf{R}_{ni}\) and \(\mathbf{R}_{en} = -\mathbf{R}_{ne},\) and heat exchange terms \(Q_{in}, Q_{en}, Q_{ni},\) and \(Q_{ne}\) can be neglected, as mentioned in section 3. Following from [5], the parameter \(\lambda,\) where \(0 \leq \lambda \leq 1,\) is introduced. If the mean free paths of the
charge-exchanged neutral particles are expected to be large, then \( \lambda \) is set between 0 and 1, so that charge-exchanged neutral particles leave the system without reacting again, taking their energy and momentum with them. If the mean free paths of the charge-exchanged neutral particles are expected to be short, then \( \lambda \) is set to zero. By default, \( \lambda \) is set to zero in the MHD simulations presented here, consistent with conservation of energy associated with the neutral fluid. The resulting set of conservation equations, in continuous form, for the two-fluid system, including ionization & recombination and charge exchange terms, as well as neutral source terms, and density diffusion (correction terms \( f_i/\rho \) and \( f_e/\rho_n \) are included to maintain energy and, in some simulation scenarios, angular momentum conservation, as described in [1, 2]), is:

\[
\dot{\rho}_i = -\nabla \cdot (\rho_i \mathbf{v}_i) + \Gamma_i^{\text{ion}} - \Gamma_i^{\text{rec}} + \nabla \cdot (\zeta \nabla n_i)
\]
\[
\dot{\mathbf{v}}_i = -\mathbf{v}_i \cdot \nabla \mathbf{v}_i + \frac{1}{\rho_i} \left( -\nabla p_i - \nabla \cdot \mathbf{\Pi}_i + \mathbf{J}_i \times \mathbf{B} - \Gamma_i^{\text{ion}} \rho_i \mathbf{v}_i - \Delta_i^{\text{ex}} \mathbf{v}_i - R_{ni}^{\text{ex}} + R_{ni}^{\text{in}} + f_i \right)
\]
\[
\dot{p}_i = -\mathbf{v}_i \cdot \nabla p_i - \gamma p_i \mathbf{v}_i \cdot \mathbf{v}_i + (\gamma - 1) \left( -\mathbf{\Pi}_i \cdot \nabla \mathbf{v}_i - \nabla \cdot \mathbf{q}_i + \eta_i' J_i^2 + \Gamma_i^{\text{ion}} \frac{1}{2} m_i v_i^2 + Q_i^{\text{ion}} - \Gamma_i^{\text{ion}} \phi_{\text{ion}} - Q_i^{\text{rec}} - Q_i^{\text{ex}} - R_{ni}^{\text{ex}} \cdot \mathbf{v}_i + Q_{ni}^{\text{ex}} - Q_{ni}^{\text{rec}} + \Gamma_i^{\text{ext}} \frac{1}{2} m_i v_i^2 \right)
\]
\[
\dot{n}_n = -\nabla \cdot (n_n \mathbf{v}_n) - \lambda \Delta^{\text{ex}} - \Gamma_i^{\text{ion}} n_i + \Gamma_i^{\text{rec}} n_i + \nabla \cdot (\zeta \nabla n_n)
\]
\[
\dot{\mathbf{v}}_n = -\mathbf{v}_n \cdot \nabla \mathbf{v}_n + \frac{1}{\rho_n} \left( -\nabla p_n - \nabla \cdot \mathbf{\Pi}_n + \gamma n_n \mathbf{v}_n - R_{in}^{\text{ex}} - (1 - \lambda) (R_{in}^{\text{ex}} + \Gamma_i^{\text{ext}} m_i \mathbf{v}_i) \right)
\]
\[
\dot{\rho}_n = -\mathbf{v}_n \cdot \nabla p_n - \gamma p_n \mathbf{v}_n \cdot \mathbf{v}_n + (\gamma - 1) \left( -\mathbf{\Pi}_n \cdot \nabla \mathbf{v}_n - \nabla \cdot \mathbf{q}_n - Q_i^{\text{ion}} + \Gamma_i^{\text{rec}} \frac{1}{2} m_i v_i^2 + Q_{i}^{\text{rec}} + \Gamma_i^{\text{ext}} \frac{1}{2} m_i v_i^2 + Q_{i}^{\text{rec}} \right)
\]
\[
+ (1 - \lambda) (R_{in}^{\text{ex}} \cdot \mathbf{v}_i + \Gamma_i^{\text{ext}} \frac{1}{2} m_i v_i^2 + Q_{in}^{\text{ex}} - Q_{in}^{\text{rec}} + \Gamma_i^{\text{ext}} \frac{1}{2} m_i (v_n - v_n)^2) \right) + \Gamma_i^{\text{ext}} \tau_n T_i
\]

The code has the option to evolve the single plasma-fluid energy equation or to evolve separate energy equations for the ions and electrons. For the latter option, when plasma-neutral interaction is included, the ion and electron energy equations are

\[
\dot{p}_i = -\mathbf{v}_i \cdot \nabla p_i - \gamma p_i \mathbf{v}_i \cdot \mathbf{v}_i + (\gamma - 1) \left( -\mathbf{\Pi}_i \cdot \nabla \mathbf{v}_i - \nabla \cdot \mathbf{q}_i + Q_{ie} + \Gamma_i^{\text{ion}} \frac{1}{2} m_i v_i^2 + Q_{i}^{\text{ion}} - Q_{i}^{\text{rec}} \right)
\]
\[
- R_{in}^{\text{ex}} \cdot \mathbf{v}_i + Q_{in}^{\text{ex}} - Q_{in}^{\text{rec}} + \Gamma_i^{\text{ext}} \frac{1}{2} m_i v_i^2 \right)
\]
\[
\dot{p}_e = -\mathbf{v}_e \cdot \nabla p_e - \gamma p_e \mathbf{v}_e \cdot \mathbf{v}_e + (\gamma - 1) \left( +\eta J_e^2 - \nabla \cdot \mathbf{q}_e - Q_{ie} - \Gamma_i^{\text{ion}} \phi_{\text{ion}} - Q_{e}^{\text{rec}} \right)
\]

where, from the Chapman-Enskog closures, neglecting the thermal force heating term, \( Q_{ei} = -Q_{ie} + \eta J^2 = -\frac{3m_e}{m_i} n_i (T_e - T_i) + \eta J^2 \). Note that \( p = p_i + p_e \), and \( \mathbf{q} = \mathbf{q}_i + \mathbf{q}_e \), so that the sum of the component energy equations yields the single plasma-fluid energy equation. The viscous term has been neglected in the electron energy equation because the magnitudes of species viscous tensor components \( (\mathbf{\Pi}_n)_{ij} \) are proportional to \( \mu_\alpha = \rho_\alpha \nu_\alpha \), where \( \mu_\alpha \), \( \rho_\alpha \), and \( \nu_\alpha \) are the dynamic viscosity, mass density, and kinematic viscosity respectively for species \( \alpha = i, e \). With \( n_i \sim n_e, T_i \sim T_e \) (recall \( \nu_\alpha \) scales with \( T_\alpha \)), and \( m_e \ll m_i \), it is reasonable to drop the viscous term from the electron energy equation.

### 7 Conservation properties with inclusion of neutral fluid

As described in [1, 2], the inherent properties of the differential operators matrices that form the core of the DELiTE code framework are used to ensure global conservation of energy, particle count, toroidal flux, and angular momentum. Because the equations for the neutral fluid are analogous, in terms of conservation properties, to the equations for the plasma fluid, it is to be expected that the conservation properties will be maintained when the evolution of a neutral fluid is simulated along with that of a plasma fluid.
Figure 1: Illustration of energy and particle conservation for MHD simulation with neutral fluid

Figure 1(a) indicates the partition of energy, and how total system energy is conserved for a simulation where a neutral fluid is evolved along with the plasma fluid. In this case, the initial neutral fluid number density was approximately equal to the initial plasma fluid number density, with spatially uniform initial distributions. The simulation started from a Grad-Shafranov equilibrium. The only explicitly applied boundary conditions were $v_r|_\Gamma = v_n|_\Gamma = v_{nr}|_\Gamma = v_{nz}|_\Gamma = 0$ and $\psi|_\Gamma = 0$, so that the thermal and Poynting fluxes are zero through the boundary, as outlined in [1, 2]. When the electron fluid energy lost through the ionization and recombination (the model assumes that in the radiative recombination reaction, the electron thermal energy is lost to the photon emitted, which leaves the optically thin system without further interaction) processes are accounted for, it is evident that total energy is conserved to numerical precision. The partitions of magnetic energy and the thermal and kinetic plasma fluid energies follow the trends outlined in [1, 2] for case without neutral fluid evolution.

Note that the neutral fluid thermal energy is negligible compared with the plasma thermal energy. Initial spatially uniform temperatures were $T_i = T_e = T_n = 0.02\text{eV}$. Due to ionization, neutral fluid density is low in regions in which electrons are hot. In these regions, ions are also generally hot due to heat exchange with electrons. The hot ions result, through the charge exchange process, in hot neutral particles, so regions with hot neutral particles are regions of relatively low neutral fluid density.

Neutral fluid kinetic energy is small compared with the kinetic energy of the ions and electrons. Charged particle acceleration leads to neutral particle acceleration, largely due to frictional forces between the plasma and neutral fluids associated with charge-exchange reactions, and due to momentum exchange arising from recombination processes. Plasma is accelerated by $\mathbf{J} \times \mathbf{B}$ forces, and is heated in regions where it is accelerated, either by ohmic heating (electrons) or viscous heating (ions). Thus, neutral fluid density tends to be low in regions where neutral fluid is accelerated due to high ionization rates in those regions, so net neutral fluid kinetic energy remains low. Figure 1(b) shows how total particle count ($N_{tot}$) is conserved to numerical precision for the same simulation. Initial neutral particle count ($N_n$) was around equal to the ion inventory ($N_i$), and by the end of the simulation, neutral particles account for around one in 100,000 of the total number of particles, due to ionization.

Net angular momentum of the plasma and neutral fluids is also conserved to numerical precision. No boundary conditions are explicitly applied to $v_\phi$ or to $v_{n\phi}$, so the natural boundary conditions $(\nabla \times \omega )|_\Gamma = (\nabla \times \omega_n )|_\Gamma = 0$ (here $\omega = v_\phi/r$ and $\omega_n = v_{n\phi}/r$ are the plasma fluid and neutral fluid angular speeds respectively) are automatically imposed, as described in [1, 2].
8 Simulation results with neutral fluid

| neutralfluid | $N_0[\text{m}^{-3}]$ | $\sigma^2_N[\text{m}^2]$ | $\zeta_n[\text{m}^2/\text{s}]$ | $\text{add}_N$ |
|--------------|----------------|----------------|----------------|-------------|
| vary$_{\text{N}}$ | vary$_{\nu\text{N}}$ | $\chi_{\text{Nmax}}[\text{m}^2/\text{s}]$ | $\nu_{\text{Nmax}}[\text{m}^2/\text{s}]$ | $\chi_{\text{CX}}$ |
| 1            | 4.5 x $10^{20}$ | 0.01           | 90             | 1           |

Table 2: Neutral-relevant code input parameters

The code inputs in table 2 are related to the neutral fluid dynamics for the simulation presented here. When interaction between the plasma and a neutral fluid is evolved, code input parameter neutralfluid is set equal to one. Analogous to the case described in [1, 2] for the initial plasma distribution, the initial static neutral fluid distribution is determined by a Gaussian profile centered around the location of the plasma injector gas valves at $z = -0.43\,\text{m}$, with variance $\sigma^2_N$ determining the degree of neutral fluid spread around the gas valves, and neutral number density scaling $N_0$. $\zeta_n[\text{m}^2/\text{s}]$ is the coefficient of neutral fluid density diffusion, which is required for numerical stability. $\text{add}_N = 1$ implies that neutral fluid is added to the simulation domain at the location of the gas valves throughout the simulation. Physically, the gas valves remain open for up to around a millisecond after they are first opened. In general, simulations including neutral dynamics have vary$_{\nu\text{N}}$ and vary$_{\chi\text{N}}$ set to one, so that the analytical closures given by the Chapman-Enskog formulae for the neutral fluid viscous and thermal diffusion coefficients are used. However, if code input $\chi_{\text{CX}}$ is also set to one, as it is for this simulation, the modified expression for $\chi_N$ is used to determine thermal diffusion for the neutral fluid:

$$\chi_n \approx \frac{75\sqrt{\pi}}{64} \frac{V_{thn}^2}{\nu_{cn} + \nu_{cx}} = \frac{75\sqrt{\pi}}{64} \frac{V_{thn}}{\lambda_{mfp} + \sigma_{cx}n_n}$$

(8.1)

This expression [4, 5] arises from the consideration that, if the charge exchange collision frequency is higher than the frequency for neutral-neutral scattering collisions, neutral thermal conductivity should be reduced. Here, $V_{thn}$ is the thermal speed of the neutral particles, $\nu_{cn} = V_{thn}/\lambda_{mfp}$ is the neutral-neutral scattering collision frequency, and $\nu_{cx} = V_{thn}/\lambda_{cx}$ is the charge exchange frequency, where $\lambda_{cx} \approx 1/(\sigma_{cx}n_n)$ is the mean free path for charge exchange collisions. According to equation 8.1, $\chi_n$ will be limited by whichever frequency dominates. If code input $\chi_{\text{CX}}$ is set to zero, $\chi_n \to (75\sqrt{\pi}/64)(V_{thn}^2/\nu_{cn})$, the standard Chapman-Enskog expression [12]. It is found that the expression in equation 8.1 results in an increase of maximum $T_n$ of around 10% compared with cases where $\chi_{\text{CX}}$ is set to zero and vary$_{\chi\text{N}}$ is set to one. Constant coefficients are used if vary$_{\nu\text{N}}$ and vary$_{\chi\text{N}}$ are set to zero. $\chi_{\text{Nmax}}$ and $\nu_{\text{Nmax}}$ determine the upper limits, required for moderately long timesteps, applied to the neutral fluid thermal and viscous diffusion coefficients.
Figure 2: Electron and neutral fluid density profiles at various times from a simulation of CT formation in the SMRT plasma injector

Figures 2(a) and (d) show the initial distributions for plasma density, represented by $n_e$, and neutral fluid density $n_n$, from a simulation of CT formation in the SMRT plasma injector, on which the magnetic compression experiment [2, 3] was conducted. The initial density distributions are Gaussian profiles, centered around the gas puff locations at $z = -0.43\text{m}$, with a higher variance for the neutral fluid distribution, representing that the neutral gas has diffused around the gas puff valve locations, while the initial plasma distribution, is more localised to the gas puff locations. The initial neutral particle inventory, determined by
$\sigma_N^2$ and $N_0$, was over half the initial plasma particle inventory for this simulation. Note that $n_e = Z_{eff} n_i$, where $Z_{eff}$, the volume-averaged ion charge, is equal to 1.3 for this simulation. Details of the models implemented to simulate CT formation, levitation and magnetic compression are presented in [1, 2]. As shown in figures 2(b) and (c), plasma is starting to enter the CT containment region at 8µs and 9µs. A front of neutral fluid precedes the plasma as it is advected upwards (figures 2(e) and (f)). Note that neutral particles are being added at the gas puff valve locations by the outer boundary at $z = -0.43m$. In the experiment, the gas valves are opened at $t \sim -400\mu s$, and remain open for $\sim 1\ms$, so that cold neutral gas is being added to the vacuum vessel throughout the simulation, at a rate that can be estimated and assigned to the simulated neutral particle source terms.

Figure 3: Electron and neutral fluid density profiles, poloidal flux contours, and ion, electron and neutral fluid temperature profiles at 8µs, from a simulation of CT formation in the SMRT plasma injector
Figures 3(a) and (b) show close-up views of $n_e$ and $n_n$ at 8$\mu$s. Figures 3(c) and (d) show $\psi$ contours and the distribution of $T_i$ at the same time. Ions are hot due to viscous heating. Ohmic heating in combination with heat exchange with ions results in hot electrons (figure 3(e)). Note that neutral fluid density is low where $T_e$ is high due ionization (figure 3(b)). Due to charge exchange reactions, neutral fluid temperature tends to equilibriise with ion temperature (figures 3 (d) and (f)), and can become hotter than ions if the thermal diffusion for neutral fluid is set to be lower than ion thermal diffusion. In general, when $\chi_{\parallel i}$ and $\chi_{\parallel e}$ are fixed at moderate experimentally relevant values such as $\chi_{\parallel e} \sim 16000$ [m$^2$/s], $\chi_{\parallel i} \sim 5000$ [m$^2$/s], $\chi_{\perp e} \sim 240$ [m$^2$/s], and $\chi_{\perp i} \sim 120$ [m$^2$/s] for this simulation, and $\chi_N$ is determined by equation 8.1, with $\chi_{N \text{ max}} \gtrsim 5 \times 10^4$, as is the case for this simulation, it is found that $T_N < T_i$.

![Figure 3](image)

Figure 3: Close-up views of $n_e$ and $n_n$ at 8$\mu$s, and $\psi$ contours and $T_i$ distribution at the same time. Due to charge exchange reactions, neutral fluid temperature tends to equilibriise with ion temperature and can become hotter than ions if the thermal diffusion for neutral fluid is set to be lower than ion thermal diffusion.

![Figure 4](image)

Figure 4: Profiles of plasma and neutral fluid axial and azimuthal velocity components at 8$\mu$s, from a simulation of CT formation in the SMRT plasma injector.

Figures 4(a) and (b) shows profiles of axial velocity at 8$\mu$s for the plasma fluid and neutral fluid respectively, while azimuthal velocity profiles are presented at the same output time in figures 4(c) and (d). Plasma acceleration leads to neutral fluid acceleration, due to frictional forces associated with charge-exchange reactions, and due to momentum exchange arising from recombination processes. It can be seen how the neutral fluid attains nearly the same velocity magnitudes as the plasma fluid.

### 8.1 Effect of inclusion of the $Q_{rec}^{e}$ term

$Q_{rec}^{e}$ [J m$^{-3}$ s$^{-1}$] determines the volumetric rate of thermal energy transfer from electrons to photons and neutral particles due to radiative recombination. As discussed in section 4.1.3, the method described in this chapter to evaluate the terms determining plasma-neutral interactions allows for the evaluation of $Q_{rec}^{e}$, which could not be evaluated by the formal moment-taking process described in [4], and has been neglected in studies [5, 18] based on the model. From looking at the kinematics of the radiative recombination reaction...
(section 4.1.3), it is more physical to neglect $Q_{\text{rec}}^e$ as an energy source for the neutral fluid (most of the electron thermal energy is transferred to the photon), but include it as an energy sink for the electron fluid. It is interesting however to note the effect of including the term as an energy source for the neutral fluid - in this (unphysical) scenario it is assumed, as presented in [4], that all the electron thermal energy lost during radiative recombination is transferred to the neutral particle.

![Figure 5: Effect of inclusion of the $Q_{\text{rec}}^e$ term, which is included in simulations pertaining to figures (a) and (b) and omitted in simulations pertaining to figures (c) and (d)](image)

Figures 5(a) and (b) show profiles of $T_n$ from a simulation in which the $Q_{\text{rec}}^e$ term is included in the energy equations for the electron and neutral fluids, at 45µs just prior to magnetic compression, and at peak compression at 65µs. Figures 5(c) and (d) show $T_n$ profiles at the same times from a simulation that is identical except that the $Q_{\text{rec}}^e$ term is not included in the plasma and neutral fluid energy equations. It can be seen how peak $T_n$ increases by around 20% at 45µs, and by around 30% at 65µs, when the $Q_{\text{rec}}^e$ term is included. Note that if $\chi_{\text{Nmax}}$ is increased from $5 \times 10^4 [\text{m}^2/\text{s}]$ to $1 \times 10^5 [\text{m}^2/\text{s}]$, that peak $T_n$ increases by around 30% at 45µs, and by around 80% at 65µs when the $Q_{\text{rec}}^e$ term is included. Not shown here, peak electron temperature falls by around 1% when the $Q_{\text{rec}}^e$ term is included. From equations 4.2, 4.3, and 4.15, it can be seen that

$$Q_{\text{rec}}^e \propto Z_{\text{eff}}^3 n_i^2 \sqrt{T_e}$$

Hence, $Q_{\text{rec}}^e$ is high in regions where plasma density and electron temperature are high. The increase in $T_n$ when $Q_{\text{rec}}^e$ is included is especially large in such regions, for example near the CT core at peak magnetic compression, where the rate of ionization is high and hence $n_n$, and thermal energy associated with neutral particles, is low.

Not shown here, peak electron temperature falls by around 1% when the $Q_{\text{rec}}^e$ term is included in the electron fluid energy equation. $Q_{\text{rec}}^e$ appears as a (physical) thermal energy sink in the electron fluid energy.
equation, but the reduction in $T_e$ when $Q_{e\text{rec}}$ is included is negligible, even in regions where $Q_{e\text{rec}}$ is high, due to the high levels of electron thermal energy in such regions.

8.2 Neutral fluid interaction in SPECTOR geometry

It is usual to observe a significant rise in electron density at around 500µs on the SPECTOR plasma injector, and it was thought that this may be a result of neutral gas, that remains concentrated around the gas valve locations after CT formation, diffusing up the gun. Ionization of the neutral particles would lead to CT fueling and an increase in observed electron density. The model for interaction between plasma and neutral fluids was applied to study the issue.

![Figure 6: Poloidal flux contours and profiles of electron and neutral fluid densities at various times from a simulation of CT formation in the SPECTOR plasma injector](image)
Figures 6(a), (b) and (c) show $\psi$ contours and profiles of $n_e$ and $n_n$ at 20\,$\mu$s, as plasma enters the CT containment region. Profiles of the same quantities are shown in figures 6(d), (e) and (f) at 500\,$\mu$s, around the time when the density rise is usually observed. It can be seen how neutral fluid density is highest at the bottom of the gun barrel (figure 6(f)) - any neutral gas advected or diffusing upwards is ionized. A region of particularly high electron density is apparent just above, and outboard of, the entrance to the containment region (figure 6(e)) - this is due to the fueling effect arising from neutral gas diffusion.

![Figure 6: Profiles of electron density and temperature at 500\,$\mu$s from a simulation of CT formation in the SPECTOR plasma injector.](image)

The region of particularly high electron density is more defined in figure 7(a), in which cross-sections of the horizontal chords representing the lines of sight of the FIR (far-infrared) interferometer [19] are also depicted. The electron temperature profile at 500\,$\mu$s is shown in figure 7(b). Referring to figure 6(f), it can be seen how neutral fluid density is low in regions of high $T_e$ as a result of ionization.

![Figure 7: Profiles of electron density and temperature at 500\,$\mu$s from a simulation of CT formation in the SPECTOR plasma injector.](image)

Figure 8: Effect of neutral fluid dynamics in SPECTOR geometry

Figure 8(a) shows line-averaged electron density measured along the interferometer chord at $r = 140$ mm from a selection of several shots in SPECTOR. It can be seen how density starts to rise at around 500 to 600\,$\mu$s. Figure 8(b) shows the simulated diagnostic for line-averaged electron density along the chords indicated in figure 7(a). The density rise is qualitatively reproduced when neutral fluid is included in the
simulation. Similar simulations without the inclusion of neutral fluid do not indicate this density rise (dashed lines in figure 8(b)). The density rise was not observed in the magnetic compression experiment because CT lifetimes were shorter than the time it takes for a sufficient amount of neutral gas to diffuse upwards toward the containment region. The simulations presented in figure 8(b) were run with artificially high plasma density in order to allow for an increased simulation timestep and moderately short simulation run-times (note that timestep scales inversely with Alfvén speed, and hence scales with $\sqrt{n_i}$ as a consequence of the explicit time-advance scheme that is implemented in the code). Note that the electron temperatures indicated in figure 7(b) are underestimations of the actual temperatures due to the overestimation of density in the simulation. The main goal of these simulations was to demonstrate that the inclusion of neutral fluid interaction can qualitatively model the observed electron density increase.

The CT fueling and cooling effect of neutral gas diffusing up the gun is thought to be related to the unusually significant increases in CT lifetime and electron temperature observed when a biased electrode was inserted 11mm into the CT edge on the SPECTOR plasma injector \[7\]. Electrode biasing involves the insertion of an electrode, that is biased relative to the vessel wall near the point of insertion, into the edge of a magnetized plasma. This leads to a radially directed electric field between the probe and the wall. The resultant $\mathbf{J} \times \mathbf{B}$ force imposed on the plasma at the edge of the CT confinement region varies with distance between the probe and the wall, because $E_r$, as well as the magnetic field, vary in that region. The associated torque overcomes viscous forces, spinning up the edge plasma, and results in shearing of the particle velocities between the probe and the wall. The sheared velocity profile is thought to suppress the growth of turbulent eddies that advect hot plasma particles to the wall, thereby reducing this plasma cooling mechanism. In general, high confinement modes induced by probe biasing share features of those initiated by various methods of heating, including a density pedestal near the wall (near the probe radius for probe biasing), diminished levels of recycling as evidenced by reduced H$\alpha$ emission intensity, and increased particle and energy confinement times.

In contrast to most of the biasing experiments conducted on tokamak plasmas, where electron density is found to increase as a consequence of biasing, electron density was markedly reduced in the SPECTOR edge biasing experiment. This density reduction is thought to be due to the effect of the transport barrier impeding the CT fueling associated with neutral gas diffusing up the gun. CT lifetimes and temperatures were found to increase by factors of around 2.4 with edge biasing. The scale of the improvements observed is significantly greater than that associated with prior biasing experiments, and it is thought that this result is associated with a reduction of the cooling effect associated with CT fueling.

9 Conclusions

It has been shown how the terms that determine the source rates of species momentum and energy due to ionization and recombination can be derived from basic principles rather than the more formal and involved process of taking successive moments of the collision operators pertaining to the reactions. The moment-taking method must be used to determine terms relating to charge exchange reactions. Only the simple method enables determination of $Q_{rec}^e$, which prescribes the volumetric rate of thermal energy transfer from electrons to photons and neutral particles due to radiative recombination. From looking at the kinematics of the radiative recombination reaction, it appears reasonable to neglect $Q_{rec}^e$ as an energy source for the neutral fluid (most of the electron thermal energy is transferred to the photon), but include it as an energy sink for the electron fluid. Inclusion of this term in the electron energy equation leads to an insignificant reduction in electron fluid temperature in the regime examined. The source rate terms have been used to develop the three fluid, and two fluid equations for plasma and neutral gas, which have been implemented to the DELiTE code framework.

Energy conservation is maintained with the inclusion of the neutral fluid model if the electron thermal energy expended on ionization and recombination processes is accounted for. The initial motivation for the study of plasma/neutral interaction was that inclusion of a neutral model was expected to lead to net ion cooling; this concept has been disproved. Increased net initial particle inventory results in lower ion temperatures, regardless of whether part of the initial inventory includes neutral particles. Charge exchange reactions lead to ion-neutral heat exchange, but the ion temperature is relatively unchanged by charge exchange reactions in hot-ion regions where electron temperature and ionization rates are also high and neutral fluid density is consequently low. The effect of residual neutral gas, that is concentrated around
the gas valves after the formation process, diffusing up the gun to the CT containment area at relatively late times in SPECTOR geometry, leading to increases in measured CT electron density, can be captured by the model. This insight helps account for the exceptionally significant increase in electron temperature, and markedly reduced electron density, observed during the electrode edge biasing experiment conducted on SPECTOR [7]. The model implementation is a good testbed for further studies and improvements.

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