LLNL-JRNL-546455

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

A General Nonlinear Fluid Model for Reacting Plasma-Neutral Mixtures

E. T. Meier, U. Shumlak

April 10, 2012

Physics of Plasmas

Disclaimer

A general nonlinear fluid model for reacting plasma-neutral mixtures

E.T. Meier

*Lawrence Livermore National Laboratory, Livermore, California 94551, USA**

U. Shumlak

Plasma Science and Innovation Center,

University of Washington, Seattle, Washington 98195-2250, USA

(Dated: June 4, 2012)

Abstract

A generalized, computationally tractable fluid model for capturing the effects of neutral particles in plasmas is derived. The model derivation begins with Boltzmann equations for singly-charged ions, electrons, and a single neutral species. Electron-impact ionization, radiative recombination, and resonant charge exchange reactions are included. Moments of the reaction collision terms are detailed. Moments of the Boltzmann equations for electron, ion, and neutral species are combined to yield a two-component plasma-neutral fluid model. Separate density, momentum, and energy equations, each including reaction transfer terms, are produced for the plasma and neutral equations. The required closures for the plasma-neutral model are discussed.

* meier23@llnl.gov

I. INTRODUCTION

A plasma-neutral model is developed in which, essentially, a single-fluid magnetohydrodynamic (MHD) plasma reacts and interacts with a gasdynamic neutral fluid. The model accounts for electron-impact ionization, radiative recombination, and resonant charge exchange (CX):

$$\begin{aligned} e^- + n &\rightarrow i^+ + 2e^- - \phi_{ion} \\ e^- + i^+ &\rightarrow n + h\nu \\ i^+ + n &\rightarrow n + i^+ \end{aligned} \tag{1}$$

The plasma-neutral model is derived from the ion, electron, and neutral species Boltzmann equations using the same basic approach as Braginskii [1], except that a neutral species is included, species conversion (due to ionization, recombination, and CX) is allowed, and related effects on mass, momentum, and energy equations are captured. Single ionization and overall charge neutrality are assumed, and electron mass is neglected. Only one type of atom, along with its associated ion, is considered. The model allows separate densities, temperatures, and velocities for the plasma and neutral fluids. An optically thin plasma is assumed so that radiation energy due to atomic physics effects, such as de-excitation energy associated with radiative recombination, is lost from the system. To simplify the model, excited states are not tracked. Instead, an effective ionization potential, ϕ_{ion}, is assumed. This potential includes the electron binding energy plus the excitation energy that is expended (on average) for each ionization event.

Background information and motivation for this research is presented in Section II. The model derivation is given in Section III. The derivation is split into four subsections. Moments of the collision operators are presented in Section III A. Mass, momentum, and energy equations are derived for ion, electron and neutral fluids in Section III B. These equations are reduced to a two-component plasma-neutral model in Section III C. Finally, in Section III D, the closures required for the plasma-neutral model are discussed. Although some specific closure options are presented, general closure remains a topic of future research. In Section IV, conclusions are drawn.

II. BACKGROUND AND MOTIVATION

In a seminal 1965 paper, Braginskii [1] derives plasma fluid equations by taking moments of ion and electron Boltzmann equations and closes the model by using the Chapman-Enskog successive-approximation method to determine the local distribution function. Braginskii's 1965 paper includes a "multicomponent plasma" model; his model treats the plasma and neutral as a combined fluid, and does allow for reactions between species and associated species conversion. For a strongly collisional plasma-neutral mixture, the combined-fluid approach of Braginskii is convenient.

Several models have been developed to simulate the interaction of the solar wind with the local interstellar medium, as discussed in the review by Zank [2]. Pauls et al. [3] describe a nonlinear two-component hydrogen ion-neutral model that meticulously accounts for CX between hydrogen ions and neutrals, but no other reactions are included. An electron species is not evolved, and electromagnetic fields are neglected. Closure is handled by assuming Maxwellian fluids. Baranov and Malama [4] present a steady state model that uses a Monte Carlo approach for handling collision integrals. Recently, a linear two-component plasma-neutral model, but without reactions and associated species conversion, is presented by Zaqarashvili et al. [5] for astrophysical plasma applications.

A variety of simulation tools have been developed to understand and predict behavior of edge plasmas in tokamaks and other fusion-grade plasmas. Two leading examples are UEDGE [6–8] and B2 [9, 10]. These codes are based on a fluid description and are often coupled to Monte Carlo neutral transport codes such as DEGAS 2 [11], and EIRENE [12]. Also, to determine turbulent transport, these 2D codes are sometimes coupled to 3D fluid codes. For example, UEDGE has been coupled to the turbulent transport code, BOUT [13]. Furthermore, these codes have been developed to treat impurity effects. Izzo et al. [14, 15] have developed an extension of the 3D NIMROD code called NIMRAD to model massive injection of impurity gas, which is used to quench tokamak disruptions. 0D and 1D models have been developed by You [16] to model refueling physics in tokamak-like devices.

A model proposed by Helander et al. [17], again aimed at magnetic fusion applications, uses a fluid moment approach similar to Braginskii to derive a combined-fluid ion-neutral model. (The electron fluid is not included in the analysis by Helander et al. In an implementation of this model, an electron fluid equation would be either solved separately or included with the ion fluid.) The neutral and ion distribution functions are assumed to be strongly coupled via CX, and a detailed description of the related closures is given.

The development of models for partially ionized gas has primarily focused on specific problems like tokamak edge physics or the interaction of the solar wind with the heliopause. A model suitable for capturing the primary fluid effects of ionization, recombination, and charge exchange in a variety of plasma science problems is not described in literature. Such a model is the objective of the research presented here.

III. PLASMA-NEUTRAL MODEL DERIVATION

This derivation is split into four parts: in Section III A, the required integrals of the collision operators are detailed; in Section III B, the three-component electron-ion-neutral model is described; in Section III C, the three-component model is reduced to the two-component plasma-neutral model; finally, in Section III D, closure of the plasma-neutral model is discussed.

The Boltzmann equation for species α is

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_\alpha + \frac{q_\alpha}{m_\alpha}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_\alpha = \left.\frac{\partial f_\alpha}{\partial t}\right|_{collisions} = C_\alpha^{scat.,react.}, \tag{2}$$

where the subscript of the collision operators, $C_\alpha^{scat.,react.}$, refers to the species affected by the term, and the superscript refers to the scattering or reacting collision type. The scattering collisions are elastic. The reactions can be thought of as inelastic collisions (except for resonant CX, in which case the initial and final quantum states are degenerate). All of the relevant collisions may be summarized as

$$\sum_{\alpha=i,e,n}\left(\sum_{scat.=ii,ie,in,ee,en,nn} C_\alpha^{scat.} + \sum_{react.=ion,rec,cx} C_\alpha^{react.}\right), \tag{3}$$

where contributions are to ion, electron, and neutral (i, e, and n) species due to scattering collisions — ion-ion, ion-electron, ion-neutral, electron-electron, electron-neutral, and neutral-neutral (ii, ie, in, ee, en, nn) — and reacting collisions — ionization, recombination, and CX (ion, rec, cx). The plasma-neutral model is derived from Eqn. (2) using the same basic approach as Braginskii [1], except that a neutral species is included, species conversion (due to ionization, recombination, and CX) is allowed, and related effects on mass, momentum, and energy equations are captured assuming reacting Maxwellian populations. As discussed in Section III D, closure of the model is achieved by adopting the results of earlier work [1, 18] that applied the Chapman-Enskog successive-approximation approach to determine local ion, electron, and neutral distribution functions.

A. Moments of collision operators

For the purposes of this derivation, specific forms of the scattering collision operators are not needed. The electron-impact ionization, radiative recombination, and resonant CX collision operators are

$$C_n^{ion} = -f_n \int f_e \sigma_{ion} v_{rel} d\mathbf{v}, \tag{4}$$

$$C_e^{ion} = C_i^{ion} = f_n \int f_e \sigma_{ion} v_{rel} d\mathbf{v}, \tag{5}$$

$$C_e^{rec} = -f_e \int f_i \sigma_{rec} v_{rel} d\mathbf{v}, \tag{6}$$

$$C_i^{rec} = -f_i \int f_e \sigma_{rec} v_{rel} d\mathbf{v}, \tag{7}$$

$$C_n^{rec} = \frac{m_e}{m_n} f_e \int f_i \sigma_{rec} v_{rel} d\mathbf{v} + \frac{m_i}{m_n} f_i \int f_e \sigma_{rec} v_{rel} d\mathbf{v}, \tag{8}$$

$$C_i^{cx} = f_n \int \sigma_{cx} v_{rel} f_i d\mathbf{v} - f_i \int \sigma_{cx} v_{rel} f_n d\mathbf{v}, \tag{9}$$

and

$$C_n^{cx} = \frac{m_i}{m_n} f_i \int \sigma_{cx} v_{rel} f_n d\mathbf{v} - \frac{m_i}{m_n} f_n \int \sigma_{cx} v_{rel} f_i d\mathbf{v}. \tag{10}$$

Here, v_{rel} is the relative speed of the colliding particles. The ionization and recombination cross-sections are assumed to be functions of only the random component of the electron particle velocity. As discussed by Ripken and Fahr [19], the form of the resonant CX collision operator is attributable to the the fact that the initial and final quantum mechanical states have identical energy. The CX cross section is assumed to be a function of a representative collision velocity as discussed below.

A Maxwellian form for f_α is assumed — $f_\alpha = n_\alpha \left(\pi v_{T\alpha}^2\right)^{-3/2} e^{-(\mathbf{v}-\mathbf{v}_\alpha)^2/v_{T\alpha}^2}$, where n_α is the species number density, $\mathbf{v}$ is the velocity, and $\mathbf{v}_\alpha$ is the species bulk velocity. The species thermal velocity is $v_{T\alpha} \equiv \sqrt{2kT_\alpha/m_\alpha}$, where T_α is the species temperature, and k is the Boltzmann constant. The random velocity is defined as $\mathbf{w} \equiv \mathbf{v} - \mathbf{v}_\alpha$.

0^{th}, 1^{st}, and 2^{nd} moments of the reaction collision operators are derived next. A summary of results is provided following the moment derivations.

As noted in Section II, Pauls et al. [3] describe these moments for resonant CX, but not for electron-impact ionization and radiative recombination. In the model proposed by Helander et al. [17], moments of the ionization and recombination collision operators are shown without supporting details. Moments of the CX operator are not necessary in the combined-fluid formulation of Helander et al. The UEDGE [6–8] and B2 [9, 10] codes can rely on Monte Carlo calculations to include the effects of reaction collisions, or use fluid models for flows parallel to the magnetic field to account for momentum and energy exchange due to ionization, recombination, and CX (though, for CX, only the direct transfer of momentum between ion and neutral fluids, as discussed below, is included).

0^{th} moments — $\int C_\alpha^{scat.,react.} d\mathbf{v}$

Scattering has no 0^{th} moment effect.

For the 0^{th} moment effect of ionization on the neutral species, the required integral of Eqn. (4) is

$$\int C_n^{ion} d\mathbf{v} = -\int f_n(\mathbf{v}') \int f_e(\mathbf{v}) \sigma_{ion}(v_{rel}) v_{rel} d\mathbf{v} d\mathbf{v}'. \tag{11}$$

Consider the inner integral over electron particle velocity space. The Maxwellian electron distribution is a function of the random velocity, $\mathbf{w} \equiv \mathbf{v} - \mathbf{v}_e$. The relative velocity is $v_{rel} = |\mathbf{v} - \mathbf{v}'|$. Assuming that the electron thermal speed is high compared to the relative fluid flow speed, $|\mathbf{v}_e - \mathbf{v}_n|$, and the neutral thermal speed, the relative velocity in the ionizing collisions is $v_{rel} \approx w$, where $w \equiv |\mathbf{w}|$. The inner integral is then

$$\int f_e(\mathbf{v}) \sigma_{ion}(v_{rel}) v_{rel} d\mathbf{v} \approx \int f_e(\mathbf{w}) \sigma_{ion}(w) w d\mathbf{w} = n_e \langle \sigma_{ion} v_e \rangle, \tag{12}$$

where $\langle \cdot \rangle$ refers to the statistical average over velocity space, and $\langle \sigma_{ion} v_e \rangle$ is the ionization rate parameter with units of volume per time. As discussed in Section III D, $\langle \sigma_{ion} v_e \rangle$ is parameterized in terms of T_e. The entire integral is now

$$\int C_n^{ion} d\mathbf{v} \approx \Gamma_n^{ion} \equiv -\int f_n(\mathbf{v}') n_e \langle \sigma_{ion} v_e \rangle d\mathbf{v}' = -n_e n_n \langle \sigma_{ion} v_e \rangle, \tag{13}$$

where the notation, $\Gamma_\alpha^{react.}$, is introduced for source rates due to a given reaction collision (*react.*) affecting species α. Using a similar procedure, the ionization contribution to the ion species is found to be $\int C_i^{ion} d\mathbf{v} \approx \Gamma_i^{ion} = -\Gamma_n^{ion}$. The ionization contribution to the electron species is identical, $\int C_e^{ion} d\mathbf{v} \approx \Gamma_e^{ion} = \Gamma_i^{ion}$. Only Γ_i^{ion} will be used to refer to ionization source rates for the ion, neutral, and electron species. Appropriate substitutions will be made based on $\Gamma_e^{ion} = -\Gamma_n^{ion} = \Gamma_i^{ion}$.

For recombination, again assuming high electron thermal speed compared to the relative bulk fluid flow speed, $|\mathbf{v}_e - \mathbf{v}_i|$, and the ion thermal speed,

$$\int C_i^{rec} d\mathbf{v} \approx \Gamma_i^{rec} \equiv -n_i n_e \langle \sigma_{rec} v_e \rangle. \tag{14}$$

The quantity $\langle\sigma_{rec}v_e\rangle$ is the recombination rate parameter. As discussed in Section III D, $\langle\sigma_{rec}v_e\rangle$ is parameterized in terms of T_e. The 0^{th} moment recombination contribution to the electron and neutral species are $\int C_e^{rec}d\mathbf{v} \approx \Gamma_e^{rec} = \Gamma_i^{rec}$ and $\int C_n^{rec}d\mathbf{v} \approx \Gamma_n^{rec} = -\Gamma_i^{rec}$. Substitutions will be made so that only Γ_n^{rec} will be used to refer to recombination source rates.

It is intuitively obvious that CX does not result in a net change of total electron, ion, or neutral populations. However, understanding the details of the CX collision term is important for higher moments and so the 0^{th} moment is examined now. Following Paul et al. [3], C_i^{cx}, given by Eqn. (9), can be accurately approximated as

$$C_i^{cx} \approx \sigma_{cx}\left(v_i^* n_i f_n - v_n^* n_n f_i\right), \tag{15}$$

where $v_\alpha^* \equiv v_{T\alpha}\sqrt{4/\pi + x^2}$. Here, $x \equiv |\mathbf{v} - \mathbf{v}_\alpha|/v_{T\alpha}$. After an additional approximation (resulting in a total worst-case error on the order of a few percent), the 0^{th} moment integration of the first term of Eqn. (15) yields

$$\int \sigma_{cx} v_i^* n_i f_n d\mathbf{v} \approx \sigma_{cx}(V_{cx}) n_i n_n V_{cx}, \tag{16}$$

where a representative speed for the CX interaction, V_{cx}, is defined as

$$V_{cx} \equiv \sqrt{\frac{4}{\pi}v_{Ti}^2 + \frac{4}{\pi}v_{Tn}^2 + v_{in}^2}, \tag{17}$$

where $v_{in}^2 \equiv |\mathbf{v}_i - \mathbf{v}_n|^2$. Note that σ_{cx} is evaluated at V_{cx}. The steps required to arrive at Eqns. (15) and (16) are detailed in the dissertation by Meier [20], which also discusses formulas for the dependence of σ_{cx} on velocity for hydrogenic species. It is useful to define the quantity

$$\Gamma^{cx} \equiv \sigma_{cx}(V_{cx}) n_i n_n V_{cx}. \tag{18}$$

Now it is clear that $\int C_i^{cx}d\mathbf{v} \approx \Gamma^{cx} - \Gamma^{cx} = 0$ and $\int C_n^{cx}d\mathbf{v} \approx m_i/m_n(\Gamma^{cx} - \Gamma^{cx}) = 0$.

1^{st} *moments* — $\int m_\alpha \mathbf{v} C_\alpha^{scat.,react.} d\mathbf{v}$

For scattering collisions affecting species α, 1^{st} moments are $\int m_\alpha \mathbf{v} C_\alpha^{scat.} d\mathbf{v}$. Splitting the particle velocity into bulk and random components, $\mathbf{v} = \mathbf{v}_\alpha + \mathbf{w}$,

$$\int m_\alpha \mathbf{v} C_\alpha^{scat.} d\mathbf{v} = m_\alpha \mathbf{v}_\alpha \int C_\alpha^{scat.} d\mathbf{v} + m_\alpha \int \mathbf{w} C_\alpha^{scat.} d\mathbf{v}. \tag{19}$$

The first term on the right is zero. The second term is the frictional force,

$$\mathbf{R}_\alpha^{scat.} = m_\alpha \int \mathbf{w} C_\alpha^{scat.} d\mathbf{v}. \tag{20}$$

Approximations of frictional forces between ions and electrons are presented by Braginskii [1]. Frictional forces between charged species (ions and electrons) and the neutral species are presented in the three-component and two-component models of Sections III B and III C, but in the closures discussed in Section III D, these terms are assumed to be negligible.

The effect of ionization on the ion species is found by taking the 1^{st} moment of Eqn. (5),

$$\int m_i \mathbf{v} C_i^{ion} d\mathbf{v} = \int m_i \mathbf{v} f_n(\mathbf{v}) \int f_e(\mathbf{v}') \sigma_{ion} v_{rel} d\mathbf{v}' d\mathbf{v}. \tag{21}$$

Using the earlier result of Eqn. (12) for the inner integral, and splitting the neutral particle velocity into bulk and random components, $\mathbf{v} = \mathbf{v}_n + \mathbf{w}$,

$$\int m_i \mathbf{v} C_i^{ion} d\mathbf{v} \approx m_i \mathbf{v}_n \Gamma_i^{ion}. \tag{22}$$

(Note that the integral of the odd function that arises in the preceding integral, and in several following integrals, vanishes.) Similarly, the 1^{st} moment contributions of ionization to the electron and neutral species are $\int m_e \mathbf{v} C_e^{ion} d\mathbf{v} \approx m_e \mathbf{v}_n \Gamma_i^{ion}$, and $\int m_n \mathbf{v} C_n^{ion} d\mathbf{v} \approx -m_n \mathbf{v}_n \Gamma_i^{ion}$.

1^{st} moment contributions of recombination to the ion, electron, and neutral species are $\int m_i \mathbf{v} C_i^{rec} d\mathbf{v} \approx -m_i \mathbf{v}_i \Gamma_n^{rec}$, $\int m_e \mathbf{v} C_e^{rec} d\mathbf{v} \approx -m_e \mathbf{v}_e \Gamma_n^{rec}$, and $\int m_n \mathbf{v} C_n^{rec} d\mathbf{v} \approx (m_i \mathbf{v}_i + m_e \mathbf{v}_e) \Gamma_n^{rec}$.

For CX, the 1^{st} moment contribution to the ion species is

$$\begin{aligned}
\int m_i \mathbf{v} C_i^{cx} d\mathbf{v} &\approx m_i \sigma_{cx} \int \mathbf{v} \left(n_i v_i^* f_n - n_n v_n^* f_i \right) d\mathbf{v} \\
&= m_i \sigma_{cx} \left(n_i \mathbf{v}_n \int v_i^* f_n d\mathbf{v} + n_i \int \mathbf{w} v_i^* f_n d\mathbf{v} - n_n \mathbf{v}_i \int v_n^* f_i d\mathbf{v} - n_n \int \mathbf{w} v_n^* f_i d\mathbf{v} \right) \\
&= m_i (\mathbf{v}_n - \mathbf{v}_i) \Gamma^{cx} + m_i \sigma_{cx} \left(n_i \int \mathbf{w} v_i^* f_n d\mathbf{v} - n_n \int \mathbf{w} v_n^* f_i d\mathbf{v} \right).
\end{aligned} \tag{23}$$

The final two terms in the last line of Eqn. (23) represent the frictional transfer of momentum, $\mathbf{R}_{in}^{cx} \equiv m_i \sigma_{cx} n_i \int \mathbf{w} v_i^* f_n d\mathbf{v}$ and $\mathbf{R}_{ni}^{cx} \equiv m_i \sigma_{cx} n_n \int \mathbf{w} v_n^* f_i d\mathbf{v}$. As found by Pauls et al. [3] (and detailed by Meier [20]), appropriate approximations for these frictional forces are

$$\mathbf{R}_{in}^{cx} \approx -m_i \sigma_{cx}(V_{cx}) n_i n_n \mathbf{v}_{in} v_{Tn}^2 \left[4 \left(\frac{4}{\pi} v_{Ti}^2 + v_{in}^2 \right) + \frac{9\pi}{4} v_{Tn}^2 \right]^{-1/2}, \tag{24}$$

and

$$\mathbf{R}_{ni}^{cx} \approx m_i \sigma_{cx}(V_{cx}) n_i n_n \mathbf{v}_{in} v_{Ti}^2 \left[4 \left(\frac{4}{\pi} v_{Tn}^2 + v_{in}^2 \right) + \frac{9\pi}{4} v_{Ti}^2 \right]^{-1/2}. \tag{25}$$

Thus, the 1^{st} moment CX contribution to the ion species is

$$\int m_i \mathbf{v} C_i^{cx} d\mathbf{v} \approx m_i (\mathbf{v}_n - \mathbf{v}_i) \Gamma^{cx} + \mathbf{R}_{in}^{cx} - \mathbf{R}_{ni}^{cx}. \tag{26}$$

The neutral species CX contribution has the same magnitude, but the opposite sign, $\int m_n \mathbf{v} C_n^{cx} d\mathbf{v} = -\int m_i \mathbf{v} C_i^{cx} d\mathbf{v} \approx m_i (\mathbf{v}_i - \mathbf{v}_n) \Gamma^{cx} + \mathbf{R}_{ni}^{cx} - \mathbf{R}_{in}^{cx}$.

The 1^{st} moment terms involving reaction rates (Γ_α^{rxn}) times velocities represent the direct transfer of momentum due to bulk fluid effects. The terms $\mathbf{R}_{in}^{cx}$ and $\mathbf{R}_{ni}^{cx}$ represent the "frictional" drag forces due to charge exchange, and are analogous to the frictional drag force acting on electrons and represented by $\eta \mathbf{j}$ in the generalized Ohm's law (see Sections III C and III D). Such frictional terms do not arise for ionization and recombination because, for those reactions, the electron thermal speed is assumed to be much faster than the relative particle motion.

2^{nd} moments — $\int \frac{1}{2} m_\alpha v^2 C_\alpha^{scat.,react.} d\mathbf{v}$

For scattering collisions between species α and β, 2^{nd} moments are $\int \frac{1}{2} m_\alpha v^2 C_\alpha^{scat.} d\mathbf{v}$. Splitting the particle velocity into bulk and random components, $\mathbf{v} = \mathbf{v}_\alpha + \mathbf{w}$,

$$\int \frac{1}{2} m_\alpha v^2 C_\alpha^{scat.} d\mathbf{v} = m_\alpha \mathbf{v}_\alpha \cdot \mathbf{R}_\alpha^{scat.} + \frac{1}{2} m_\alpha \int w^2 C_\alpha^{scat.} d\mathbf{v}, \tag{27}$$

where the first term, involving the frictional force (already discussed), represents conversion of kinetic to thermal energy, i.e., frictional heating. The second term,

$$Q_\alpha^{scat.} \equiv \frac{1}{2} m_\alpha \int w^2 C_\alpha^{scat.} d\mathbf{v}, \tag{28}$$

is called "heat generation" by Braginskii (*cf*. discussion on p. 232 of Braginskii [1]). Because $Q_\alpha^{scat.}$ is more accurately described as an inter-species exchange of energy, this term will be referred to as "heat exchange". The approach of Braginskii [1] may be followed for the terms in Eqn. (27) corresponding to ion-electron scattering. Eqn. (27) also describes charged-neutral (i.e., ion-neutral and electron-neutral) scattering collisions. Ion-electron and charged-neutral 2^{nd} moment terms are presented in the three-component model of Section III B. The ion-electron terms cancel in the reduction of the three-component model to the two-component model of Section III C. As discussed in Section III D, the charged-neutral terms can often (but certainly not always) be neglected.

The 2^{nd} moment of C_i^{ion}, after again using Eqn. (12) for the integral over electron velocity space, is

$$\int \frac{1}{2} m_i v^2 C_i^{ion} d\mathbf{v} \approx m_i n_e \langle \sigma_{ion} v_e \rangle \left(\frac{1}{2} v_n^2 \int f_n d\mathbf{v} + \frac{1}{2} \int w^2 f_n d\mathbf{v} \right). \tag{29}$$

The first term on the right is related to the 0^{th} moment. The second term is easily evaluated in spherical coordinates. Inserting the Maxwellian form for f_n, the integral is

$$\int w^2 f_n d\mathbf{v} = \frac{3}{2} n_n v_{Tn}^2, \tag{30}$$

Eqn. (29) is now

$$\int \frac{1}{2} m_i v^2 C_i^{ion} d\mathbf{v} \approx \frac{m_i}{m_n} \frac{\Gamma_i^{ion}}{2} \left(m_n v_n^2 + \frac{3}{2} m_n v_{Tn}^2 \right). \tag{31}$$

Using the definition of v_{Tn}, the two terms on the right can be identified as transfer of kinetic energy and internal energy. Defining $Q_n^{ion} \equiv \Gamma_i^{ion} \frac{3}{2} k T_n$, the equation for the 2^{nd} moment of C_i^{ion} can be expressed as

$$\int \frac{1}{2} m_i v^2 C_i^{ion} d\mathbf{v} \approx \frac{m_i}{m_n} \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right). \tag{32}$$

Similarly,

$$\int \frac{1}{2} m_e v^2 C_e^{ion} d\mathbf{v} \approx \frac{m_e}{m_n} \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right) - \Gamma_i^{ion} \phi_{ion}, \tag{33}$$

where the effective ionization energy is extracted, and

$$\int \frac{1}{2} m_n v^2 C_n^{ion} d\mathbf{v} \approx - \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right). \tag{34}$$

The 2^{nd} moment of C_i^{rec} is

$$\int \frac{1}{2} m_i v^2 C_i^{rec} d\mathbf{v} \approx - \left(\Gamma_n^{rec} \frac{1}{2} m_i v_i^2 + Q_i^{rec} \right), \tag{35}$$

where $Q_i^{rec} \equiv \Gamma_n^{rec} \frac{3}{2} k T_i$. The 2^{nd} moment of C_e^{rec} is

$$\int \frac{1}{2} m_e v^2 C_e^{rec} d\mathbf{v} = -\frac{1}{2} m_e n_i \left(v_e^2 \int f_e \sigma_{rec} v_{rel} d\mathbf{v} + \int w^2 f_e \sigma_{rec} v_{rel} d\mathbf{v} \right). \tag{36}$$

Here, the usual high electron thermal speed assumption is made. The product $\sigma_{rec} v_{rel}$ is assumed to be independent of ion velocity, and is extracted from the inner integral of Eqn. (6). The inner integral yields the ion density, n_i, which is seen in Eqn. (36). The first term on the right side of Eqn. (36) represents transfer of kinetic energy; the integral over electron velocity space gives $n_e \langle \sigma_{rec} v_e \rangle$ just as seen for the 0^{th} moment in Eqn. (14). The second term, representing conversion of electron thermal energy, involves the integral $\int f_e \sigma_{rec} w^3 d\mathbf{v}$. Whereas the 0^{th} moment integral $\int f_e \sigma_{rec} w d\mathbf{v}$ results in $n_e \langle \sigma_{rec} v_e \rangle$, where $\langle \sigma_{rec} v_e \rangle$ is parameterized in terms of T_e, a convenient parameterization for the integral $\int f_e \sigma_{rec} w^3 d\mathbf{v}$ in Eqn. (36) is not immediately available because an additional factor of w^2 is entangled in the integral. For further discussion, see Section III D. Defining $Q_e^{rec} \equiv 1/2 m_e n_i \int f_e \sigma_{rec} w^3 d\mathbf{v}$,

$$\int \frac{1}{2} m_e v^2 C_e^{rec} d\mathbf{v} = - \left(\Gamma_n^{rec} \frac{1}{2} m_e v_e^2 + Q_e^{rec} \right). \tag{37}$$

The 2^{nd} moment of C_n^{rec} is

$$\int \frac{1}{2}m_n v^2 C_n^{rec} d\mathbf{v} \approx \Gamma_n^{rec}\left(\frac{1}{2}m_i v_i^2 + \frac{1}{2}m_e v_e^2\right) + Q_i^{rec} + Q_e^{rec}. \tag{38}$$

The 2^{nd} moment contribution of CX to the ion species is

$$\int \frac{1}{2}m_i v^2 C_i^{cx} d\mathbf{v} \approx \frac{1}{2}m_i \sigma_{cx} \int v^2 \left(v_i^* n_i f_n - v_n^* n_n f_i\right) d\mathbf{v}, \tag{39}$$

which, after expanding the velocities into fluid and random velocities, is

$$\begin{aligned}\int \frac{1}{2}m_i v^2 C_i^{cx} d\mathbf{v} \approx m_i \sigma_{cx} \Bigg(&\frac{1}{2}n_i v_n^2 \int v_i^* f_n d\mathbf{v} - \frac{1}{2}n_n v_i^2 \int v_n^* f_i d\mathbf{v} + n_i \mathbf{v}_n \cdot \int \mathbf{w} v_i^* f_n d\mathbf{v} \\ &-n_n \mathbf{v}_i \cdot \int \mathbf{w} v_n^* f_i d\mathbf{v} + \frac{1}{2}\int \mathbf{w}^2 \left(n_i v_i^* f_n - n_n v_n^* f_i\right) d\mathbf{v}\Bigg) \\ &= \Gamma^{cx}\frac{1}{2}m_i (v_n^2 - v_i^2) + \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} - \mathbf{v}_i \cdot \mathbf{R}_{ni}^{cx} \\ &+\frac{1}{2}\sigma_{cx} m_i \int w^2 \left(n_i v_i^* f_n - n_n v_n^* f_i\right) d\mathbf{v}. \end{aligned} \tag{40}$$

The integral terms in the last line of Eqn. (40) represent the transfer of random thermal energy, $Q_{in}^{cx} \equiv \frac{1}{2}\sigma_{cx} m_i \int \mathbf{w}^2 n_i v_i^* f_n d\mathbf{v}$ and $Q_{ni}^{cx} \equiv \frac{1}{2}\sigma_{cx} m_i \int \mathbf{w}^2 n_n v_n^* f_i d\mathbf{v}$. As found by Pauls et al. [3] (and detailed by Meier [20]), appropriate approximations of these thermal energy transfers are

$$Q_{in}^{cx} \approx \sigma_{cx}(V_{cx}) m_i n_i n_n \frac{3}{4} v_{Tn}^2 \sqrt{\frac{4}{\pi} v_{Ti}^2 + \frac{64}{9\pi} v_{Tn}^2 + v_{in}^2}, \tag{41}$$

and

$$Q_{ni}^{cx} \approx \sigma_{cx}(V_{cx}) m_i n_i n_n \frac{3}{4} v_{Ti}^2 \sqrt{\frac{4}{\pi} v_{Tn}^2 + \frac{64}{9\pi} v_{Ti}^2 + v_{in}^2}. \tag{42}$$

Eqn. (39) can now be written

$$\int \frac{1}{2}m_i v^2 C_i^{cx} d\mathbf{v} \approx \Gamma^{cx}\frac{1}{2}m_i (v_n^2 - v_i^2) + \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} - \mathbf{v}_i \cdot \mathbf{R}_{ni}^{cx} + Q_{in}^{cx} - Q_{ni}^{cx}. \tag{43}$$

The 2^{nd} moment of C_n^{cx} is

$$\int \frac{1}{2}m_n v^2 C_n^{cx} d\mathbf{v} \approx \Gamma^{cx}\frac{1}{2}m_i (v_i^2 - v_n^2) - \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} + \mathbf{v}_i \cdot \mathbf{R}_{ni}^{cx} - Q_{in}^{cx} + Q_{ni}^{cx}. \tag{44}$$

Summary of reaction collision operator integrals

Summarizing for the 0^{th} moment,

$$\begin{aligned} &\int C_e^{ion} d\mathbf{v} \approx \Gamma_i^{ion}, \int C_i^{ion} d\mathbf{v} \approx \Gamma_i^{ion}, \int C_n^{ion} d\mathbf{v} \approx -\Gamma_i^{ion} \\ &\int C_e^{rec} d\mathbf{v} \approx -\Gamma_n^{rec}, \int C_i^{rec} d\mathbf{v} \approx -\Gamma_n^{rec}, \int C_n^{rec} d\mathbf{v} \approx \Gamma_n^{rec} \\ &\int C_i^{cx} d\mathbf{v} \approx \Gamma^{cx} - \Gamma^{cx} = 0, \int C_n^{cx} d\mathbf{v} \approx \Gamma^{cx} - \Gamma^{cx} = 0. \end{aligned} \tag{45}$$

Summarizing for the 1^{st} moment,

$$
\begin{aligned}
&\int m_e \mathbf{v} C_e^{ion} d\mathbf{v} \approx m_e \mathbf{v}_n \Gamma_i^{ion}, \int m_i \mathbf{v} C_i^{ion} d\mathbf{v} \approx m_i \mathbf{v}_n \Gamma_i^{ion}, \int m_n \mathbf{v} C_n^{ion} d\mathbf{v} \approx -m_n \mathbf{v}_n \Gamma_i^{ion} \\
&\int m_e \mathbf{v} C_e^{rec} d\mathbf{v} \approx -m_e \mathbf{v}_e \Gamma_n^{rec}, \int m_i \mathbf{v} C_i^{rec} d\mathbf{v} \approx -m_i \mathbf{v}_i \Gamma_n^{rec}, \int m_n \mathbf{v} C_n^{rec} d\mathbf{v} \approx (m_i \mathbf{v}_i + m_e \mathbf{v}_e) \Gamma_n^{rec} \\
&\int m_i \mathbf{v} C_i^{cx} d\mathbf{v} \approx m_i \left(\mathbf{v}_n - \mathbf{v}_i\right) \Gamma^{cx} + \mathbf{R}_{in}^{cx} - \mathbf{R}_{ni}^{cx} \\
&\int m_n \mathbf{v} C_n^{cx} d\mathbf{v} \approx m_i \left(\mathbf{v}_i - \mathbf{v}_n\right) \Gamma^{cx} + \mathbf{R}_{ni}^{cx} - \mathbf{R}_{in}^{cx}.
\end{aligned} \tag{46}
$$

Summarizing for the 2^{nd} moment,

$$
\begin{aligned}
&\int \frac{1}{2} m_e v^2 C_e^{ion} d\mathbf{v} \approx \frac{m_e}{m_n} \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right) - \Gamma_i^{ion} \phi_{ion} \\
&\int \frac{1}{2} m_i v^2 C_i^{ion} d\mathbf{v} \approx \frac{m_i}{m_n} \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right) \\
&\int \frac{1}{2} m_n v^2 C_n^{ion} d\mathbf{v} \approx - \left(\Gamma_i^{ion} \frac{1}{2} m_n v_n^2 + Q_n^{ion} \right) \\
&\int \frac{1}{2} m_e v^2 C_e^{rec} d\mathbf{v} \approx - \left(\Gamma_n^{rec} \frac{1}{2} m_e v_e^2 + Q_e^{rec} \right) \\
&\int \frac{1}{2} m_i v^2 C_i^{rec} d\mathbf{v} \approx - \left(\Gamma_n^{rec} \frac{1}{2} m_i v_i^2 + Q_i^{rec} \right) \\
&\int \frac{1}{2} m_n v^2 C_n^{rec} d\mathbf{v} \approx \Gamma_n^{rec} \left(\frac{1}{2} m_i v_i^2 + \frac{1}{2} m_e v_e^2 \right) + Q_i^{rec} + Q_e^{rec} \\
&\int \frac{1}{2} m_i v^2 C_i^{cx} d\mathbf{v} \approx \Gamma^{cx} \frac{1}{2} m_i \left(v_n^2 - v_i^2 \right) + \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} - \mathbf{v}_i \cdot \mathbf{R}_{ni}^{cx} + Q_{in}^{cx} - Q_{ni}^{cx} \\
&\int \frac{1}{2} m_n v^2 C_n^{cx} d\mathbf{v} \approx \Gamma^{cx} \frac{1}{2} m_i \left(v_i^2 - v_n^2 \right) + \mathbf{v}_i \cdot \mathbf{R}_{ni}^{cx} - \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} + Q_{ni}^{cx} - Q_{in}^{cx}.
\end{aligned} \tag{47}
$$

B. Three-component electron-ion-neutral model

The next step toward the two-component plasma-neutral equations is to compose the three-fluid electron-ion-neutral model, which is a generalization of the two-fluid plasma model [21, 22] to include reacting neutrals. Using the expressions for moments of the reaction collision operators summarized in Section III A, and taking moments of Eqn. (2) (closely following the approach of Braginskii [1]), the following continuity, momentum, and energy equations are derived for the ion, electron, and neutral species.

Continuity

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}_i) = \Gamma_i^{ion} - \Gamma_n^{rec}, \tag{48}$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{v}_e) = \Gamma_i^{ion} - \Gamma_n^{rec}, \tag{49}$$

$$\frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{v}_n) = \Gamma_n^{rec} - \Gamma_i^{ion}. \tag{50}$$

Momentum

$$\frac{\partial}{\partial t}(m_i n_i \mathbf{v}_i) + \nabla \cdot (m_i n_i \mathbf{v}_i \mathbf{v}_i + \mathbb{P}_i) = q_i n_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$
$$+\mathbf{R}_i^{ie} + \mathbf{R}_i^{in} + \Gamma_i^{ion} m_i \mathbf{v}_n - \Gamma_n^{rec} m_i \mathbf{v}_i + \Gamma^{cx} m_i (\mathbf{v}_n - \mathbf{v}_i) + \mathbf{R}_{in}^{cx} - \mathbf{R}_{ni}^{cx}, \tag{51}$$

$$\frac{\partial}{\partial t}(m_e n_e \mathbf{v}_e) + \nabla \cdot (m_e n_e \mathbf{v}_e \mathbf{v}_e + \mathbb{P}_e) = -q_e n_e (\mathbf{E} + \mathbf{v}_e \times \mathbf{B})$$
$$-\mathbf{R}_i^{ie} + \mathbf{R}_e^{en} + \Gamma_i^{ion} m_e \mathbf{v}_n - \Gamma_n^{rec} m_e \mathbf{v}_e, \tag{52}$$

$$\frac{\partial}{\partial t}(m_n n_n \mathbf{v}_n) + \nabla \cdot (m_n n_n \mathbf{v}_n \mathbf{v}_n + \mathbb{P}_n) =$$
$$-\mathbf{R}_i^{in} - \mathbf{R}_e^{en} + \Gamma_n^{rec}(m_i \mathbf{v}_i + m_e \mathbf{v}_e) - \Gamma_i^{ion} m_n \mathbf{v}_n + \Gamma^{cx} m_i (\mathbf{v}_i - \mathbf{v}_n)$$
$$-\mathbf{R}_{in}^{cx} + \mathbf{R}_{ni}^{cx}, \tag{53}$$

where q_i and q_e are the ion and electron charge magnitudes, respectively, and $\mathbf{R}_i^{ie}$ is the usual scattering collisional transfer of momentum to the ion species presented by Braginskii [1] as $\mathbf{R}_{ie}$. $\mathbf{R}_i^{in}$ is a similar scattering collisional momentum transfer to the ion species, but for ion-neutral collisions. $\mathbf{R}_e^{en}$ is a similar momentum transfer for electron-neutral collisions. The species pressure tensor, $\mathbb{P}_\alpha$, can be decomposed as $\mathbb{P}_\alpha = p_\alpha \mathbb{I} + \Pi_\alpha$, where p_α is the scalar pressure and Π_α is the stress tensor.

Energy

$$\frac{\partial \varepsilon_i}{\partial t} + \nabla \cdot (\varepsilon_i \mathbf{v}_i + \mathbf{v}_i \cdot \mathbb{P}_i + \mathbf{h}_i) = \mathbf{v}_i \cdot (q_i n_i \mathbf{E} + \mathbf{R}_i^{ie} + \mathbf{R}_i^{in})$$

$$+Q_i^{ie} + Q_i^{in} + \frac{m_i}{m_n}(\Gamma_i^{ion}\frac{1}{2}m_n v_n^2 + Q_n^{ion}) - \Gamma_n^{rec}\frac{1}{2}m_i v_i^2 - Q_i^{rec}$$
$$+\Gamma^{cx}\frac{1}{2}m_i\left(v_n^2 - v_i^2\right) + \mathbf{v}_n\cdot\mathbf{R}_{in}^{cx} - \mathbf{v}_i\cdot\mathbf{R}_{ni}^{cx} + Q_{in}^{cx} - Q_{ni}^{cx}, \tag{54}$$

$$\frac{\partial\varepsilon_e}{\partial t} + \nabla\cdot(\varepsilon_e\mathbf{v}_e + \mathbf{v}_e\cdot\mathbb{P}_e + \mathbf{h}_e) = \mathbf{v}_e\cdot(-q_e n_e\mathbf{E} - \mathbf{R}_i^{ie} + \mathbf{R}_e^{en})$$
$$+Q_e^{ie} + Q_e^{en} + \frac{m_e}{m_n}(\Gamma_i^{ion}\frac{1}{2}m_n v_n^2 + Q_n^{ion}) - \Gamma_i^{ion}\phi_{ion} - \Gamma_n^{rec}\frac{1}{2}m_e v_e^2 - Q_e^{rec}, \tag{55}$$

$$\frac{\partial\varepsilon_n}{\partial t} + \nabla\cdot(\varepsilon_n\mathbf{v}_n + \mathbf{v}_n\cdot\mathbb{P}_n + \mathbf{h}_n) = -\mathbf{v}_n\cdot(\mathbf{R}_i^{in} + \mathbf{R}_e^{en})$$
$$+Q_n^{in} + Q_n^{en} + \Gamma_n^{rec}(\frac{1}{2}m_i v_i^2 + \frac{1}{2}m_e v_e^2) + Q_i^{rec} + Q_e^{rec} - (\Gamma_i^{ion}\frac{1}{2}m_n v_n^2 + Q_n^{ion})$$
$$+\Gamma^{cx}\frac{1}{2}m_i(v_i^2 - v_n^2) + \mathbf{v}_i\cdot\mathbf{R}_{ni}^{cx} - \mathbf{v}_n\cdot\mathbf{R}_{in}^{cx} + Q_{ni}^{cx} - Q_{in}^{cx}, \tag{56}$$

where $\varepsilon_\alpha \equiv m_\alpha n_\alpha v_\alpha^2/2 + p_\alpha/(\gamma-1)$ is the total fluid energy density, and Q_i^{ie} and Q_e^{ie} are the usual scattering collisional heat exchange presented by Braginskii [1] as Q_{ie} and Q_{ei}, respectively. $Q_{i/n}^{in}$ and $Q_{e/n}^{en}$ represent the same type of heat exchange due to ion-neutral and electron-neutral collisions, respectively. The species heat fluxes are represented by $\mathbf{h}_\alpha$. Maxwell's equations couple the fluid dynamics to the electric and magnetic field evolution. The heat fluxes ($\mathbf{h}_\alpha$), and the stress tensors (Π_α) must be specified to close the model. This closure is often accomplished by using a Chapman-Enskog-like determination of the local distribution functions. These terms are further addressed in Section III D.

To compare to the well-known two-fluid transport equations presented by Braginskii [1], it is useful to identify temperature evolution equations for this three-component ion-electron-neutral model. Beginning with the fluid energy evolution equations above, kinetic energy evolution is subtracted to find pressure evolution. For each species, kinetic energy evolution is found by taking the scalar product of the fluid velocity with the momentum equation. The species continuity equations are used to simplify the results. (This procedure is outlined by Braginskii [1], and is described in some detail by Meier [20].) Next, temperature evolution is isolated. For the ion species, for example, the ion continuity equation is used to find the relationship

$$\frac{1}{\gamma-1}\frac{\partial p_i}{\partial t} + \nabla\cdot\left(\frac{1}{\gamma-1}p_i\mathbf{v}_i\right) = \frac{kn_i}{\gamma-1}\left(\frac{\partial T_i}{\partial t} + \mathbf{v}_i\cdot\nabla T_i\right) + \frac{kT_i}{\gamma-1}\left(\Gamma_i^{ion} - \Gamma_n^{rec}\right). \tag{57}$$

Similar relationships for electron and neutral temperature evolution are easily found. The resulting temperature evolution equations are

$$\frac{kn_i}{\gamma-1}\left(\frac{\partial T_i}{\partial t} + \mathbf{v}_i\cdot\nabla T_i\right) + p_i\nabla\cdot\mathbf{v}_i = -\nabla\cdot\mathbf{q}_i - \Pi_i : \nabla\mathbf{v}_i - \frac{kT_i}{\gamma-1}\left(\Gamma_i^{ion} - \Gamma_n^{rec}\right)$$

$$
+Q_i^{ie} + Q_i^{in} + \left(\Gamma_i^{ion} + \Gamma^{cx}\right) \frac{m_i}{2} (\mathbf{v}_i - \mathbf{v}_n)^2 + \frac{m_i}{m_n} Q_n^{ion} - Q_i^{rec}
$$

$$
+\mathbf{R}_{in}^{cx} \cdot (\mathbf{v}_n - \mathbf{v}_i) + Q_{in}^{cx} - Q_{ni}^{cx}, \tag{58}
$$

$$
\frac{kn_e}{\gamma - 1}\left(\frac{\partial T_e}{\partial t} + \mathbf{v}_e \cdot \nabla T_e\right) + p_e \nabla \cdot \mathbf{v}_e = -\nabla \cdot \mathbf{q}_e - \Pi_e : \nabla \mathbf{v}_e - \frac{kT_e}{\gamma - 1}\left(\Gamma_i^{ion} - \Gamma_n^{rec}\right)
$$

$$
+Q_e^{ie} + Q_e^{en} + \Gamma_i^{ion}\left[\frac{m_e}{2}(\mathbf{v}_e - \mathbf{v}_n)^2 - \phi_{ion}\right] + \frac{m_e}{m_n} Q_n^{ion} - Q_e^{rec}, \tag{59}
$$

$$
\frac{kn_n}{\gamma - 1}\left(\frac{\partial T_n}{\partial t} + \mathbf{v}_n \cdot \nabla T_n\right) + p_n \nabla \cdot \mathbf{v}_n = -\nabla \cdot \mathbf{q}_n - \Pi_n : \nabla \mathbf{v}_n - \frac{kT_n}{\gamma - 1}\left(\Gamma_n^{rec} - \Gamma_i^{ion}\right)
$$

$$
+Q_n^{in} + Q_n^{en} + \Gamma_n^{rec}\left(\frac{m_i}{2} v_i^2 + \frac{m_n}{2} v_n^2 + \frac{m_e}{2} v_e^2 - m_e \mathbf{v}_n \cdot \mathbf{v}_e - m_i \mathbf{v}_n \cdot \mathbf{v}_i\right)
$$

$$
+Q_i^{rec} + Q_e^{rec} - Q_n^{ion} + \Gamma^{cx} \frac{m_i}{2} (\mathbf{v}_n - \mathbf{v}_i)^2 + \mathbf{R}_{ni}^{cx} \cdot (\mathbf{v}_i - \mathbf{v}_n)
$$

$$
+Q_{ni}^{cx} - Q_{in}^{cx}. \tag{60}
$$

C. Two-component plasma-neutral model

To reach a two-component model, the electron and ion fluids are treated as a single fluid. The MHD approximations are made, such that $n = n_i = n_e$, $m_e \to 0$, and $\mathbf{v} = \mathbf{v}_i$. It is further assumed that $q = q_i = q_e$ and $m_i = m_n$. Current density, $\mathbf{j} = qn(\mathbf{v}_i - \mathbf{v}_e)$, is introduced.

Continuity

Along with the neutral continuity equation, only a single plasma continuity equation is needed.

$$
\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = \Gamma_i^{ion} - \Gamma_n^{rec}, \tag{61}
$$

$$
\frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{v}_n) = \Gamma_n^{rec} - \Gamma_i^{ion}. \tag{62}
$$

Momentum

The ion and electron momentum equations are summed to yield the plasma momentum equation.

$$
\frac{\partial}{\partial t}(m_i n \mathbf{v}) + \nabla \cdot (m_i n \mathbf{v}\mathbf{v} + p\mathbb{I} + \Pi) = \mathbf{j} \times \mathbf{B}
$$

$$
+\mathbf{R}_i^{in} + \mathbf{R}_e^{en} + \Gamma_i^{ion} m_i \mathbf{v}_n - \Gamma_n^{rec} m_i \mathbf{v} + \Gamma^{cx} m_i (\mathbf{v}_n - \mathbf{v}) + \mathbf{R}_{in}^{cx} - \mathbf{R}_{ni}^{cx}, \tag{63}
$$

$$\frac{\partial}{\partial t}(m_i n_n \mathbf{v}_n) + \nabla \cdot (m_i n_n \mathbf{v}_n \mathbf{v}_n + p_n \mathbb{I} + \Pi_n) =$$
$$-\mathbf{R}_i^{in} - \mathbf{R}_e^{en} + \Gamma_n^{rec} m_i \mathbf{v} - \Gamma_i^{ion} m_i \mathbf{v}_n + \Gamma^{cx} m_i (\mathbf{v} - \mathbf{v}_n) + \mathbf{R}_{ni}^{cx} - \mathbf{R}_{in}^{cx}. \tag{64}$$

To arrive at Eqn. (63) for plasma momentum evolution, the relationship [1, 23, 24]

$$m_i n \mathbf{v}\mathbf{v} + \mathbb{P} = \sum_{\alpha=i,e} (m_\alpha n \mathbf{v}_\alpha \mathbf{v}_\alpha + \mathbb{P}_\alpha)$$

is used. The total scalar plasma pressure is $p = p_i + p_e$, and the total plasma stress tensor is $\Pi = \Pi_i + \Pi_e$. Assuming the same density and temperature for ions and electrons, for magnetized or unmagnetized plasma, the components of the electron stress tensor, Π_e, are all much smaller than the corresponding components in the ion stress tensor, Π_i, essentially because of the much larger momentum carried by ions [1]. Components of Π_e are smaller than the corresponding components of Π_i by a factor of $\sqrt{m_i/m_e}$ or greate r. The factor $\sqrt{m_i/m_e}$ is approximately 43 for protons and is larger for species with higher atomic numbers, so the approximation $\Pi \approx \Pi_i$ is appropriate.

Generalized Ohm's law

The generalized Ohm's law is found from the electron momentum equation after letting $m_e \to 0$, and using $\mathbf{v}_e = \mathbf{v}_i - \mathbf{j}/qn$, where $\mathbf{j}$ is defined in terms of $\mathbf{B}$ via the low-frequency Ampère's law.

$$\mathbf{E} + \mathbf{v} \times \mathbf{B} = \frac{1}{qn}\left(\mathbf{j} \times \mathbf{B} - \nabla \cdot \mathbb{P}_e - \mathbf{R}_i^{ie} + \mathbf{R}_e^{en}\right).$$

Applying Faraday's law, this can be written as

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left[\mathbf{v} \times \mathbf{B} - \frac{1}{qn}\left(\mathbf{j} \times \mathbf{B} - \nabla \cdot \mathbb{P}_e - \mathbf{R}_i^{ie} + \mathbf{R}_e^{en}\right)\right]. \tag{65}$$

Energy

Again adding the electron and ion equations and letting $m_e \to 0$,

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{v} + \mathbf{v} \cdot (p\mathbb{I} + \Pi) + \mathbf{h}) =$$
$$\mathbf{j} \cdot \mathbf{E} + \mathbf{v} \cdot \mathbf{R}_i^{in} + \mathbf{v}_e \cdot \mathbf{R}_e^{en} + Q_i^{in} + Q_e^{en}$$
$$+\Gamma_i^{ion}\left(\frac{1}{2} m_i \mathbf{v}_n^2 - \phi_{ion}\right) + Q_n^{ion} - \Gamma_n^{rec}\frac{1}{2} m_i \mathbf{v}^2 - Q_i^{rec} - Q_e^{rec}$$
$$+\Gamma^{cx}\frac{1}{2} m_i \left(\mathbf{v}_n^2 - \mathbf{v}^2\right) + \mathbf{v}_n \cdot \mathbf{R}_{in}^{cx} - \mathbf{v} \cdot \mathbf{R}_{ni}^{cx} + Q_{in}^{cx} - Q_{ni}^{cx}, \tag{66}$$

$$\frac{\partial \varepsilon_n}{\partial t} + \nabla\cdot(\varepsilon_n \mathbf{v}_n + \mathbf{v}_n\cdot(p_n\mathbb{I} + \Pi_n) + \mathbf{h}_n) = -\mathbf{v}_n\cdot(\mathbf{R}_i^{in} + \mathbf{R}_e^{en})$$
$$+Q_n^{in} + Q_n^{en} + \Gamma_n^{rec}\frac{1}{2}m_i\mathbf{v}^2 + Q_i^{rec} + Q_e^{rec} - \Gamma_i^{ion}\frac{1}{2}m_i\mathbf{v}_n^2 - Q_n^{ion}$$
$$+\Gamma^{cx}\frac{1}{2}m_i(\mathbf{v}^2 - \mathbf{v}_n^2) + \mathbf{v}\cdot\mathbf{R}_{ni}^{cx} - \mathbf{v}_n\cdot\mathbf{R}_{in}^{cx} + Q_{ni}^{cx} - Q_{in}^{cx}. \tag{67}$$

To arrive at Eqn. (66) for plasma fluid energy evolution, $\mathbf{R}_i^{ie}\cdot(\mathbf{v}-\mathbf{v}_e)$ has cancelled with $Q_i^{ie}+Q_e^{ie}$ as discussed by Braginskii [1]. The relationship [1, 23, 24]

$$\varepsilon\mathbf{v} + \mathbf{v}\cdot\mathbb{P} + \mathbf{h} = \sum_{\alpha=i,e}(\varepsilon_\alpha\mathbf{v}_\alpha + \mathbf{v}_\alpha\cdot\mathbb{P}_\alpha + \mathbf{h}_\alpha)$$

is used in adding the ion and electron flux terms. Here, $\varepsilon = (p_i + p_e)/(\gamma - 1) + \rho v^2/2$, and $\mathbf{h} = \mathbf{h}_i + \mathbf{h}_e - \gamma p_e \mathbf{j}/[ne(\gamma - 1)]$. (The electron stress tensor is neglected in defining $\mathbf{h}$.)

Alternative formulations of the energy equations may be desired. For example, Meier [20] derives equations for plasma and neutral species pressure evolution.

D. Closure of plasma-neutral model

In general, when taking moments of Boltzmann equations to generate fluid moment equations, each moment produces terms that depend on the next higher moment of the distribution function. The fluid moment procedure must be "closed" by using a limited set of fluid equations to approximately determine each species distribution function. For the three-component electron-ion-neutral and two-component plasma-neutral models derived above, the moment procedure is truncated after the second moment. Closure is established by applying the Chapman-Enskog approach as discussed in detail by Braginskii [1]. The species distribution functions are expanded as $f_\alpha = f_\alpha^0 + f_\alpha^1 + f_\alpha^2 + \cdots$, where f_α^0 is Maxwellian, and the additional terms represent higher-order perturbations. Typically, only the first-order perturbations (f_α^1) are retained. Braginskii [1] describes the closure of his plasma models under the assumption that the lowest-order terms in the ion and electron Boltzmann equations are the scattering collision terms and the magnetic terms. The same assumption is adopted for the closures suggested here for the plasma-neutral model. Other researchers have assumed different orderings. For example, Helander et al. [17] assume that CX collision terms are dominant in the neutral species Boltzmann equation. As discussed by Meier [20], a generalization that allows scattering, CX, ionization, and recombination reactions to share the dominant role is an objective of future research.

The higher-order terms generated by the moment procedure are the heat fluxes ($\mathbf{h}_\alpha$) and stress tensors (Π_α). Once the distribution functions have been approximated, these terms can be quantified. The presence of non-Maxwellian perturbations to the distribution functions also has implications for moments of the collision operators. For example, Braginskii [1] discusses and quantifies the thermal gradient force that contributes to the ion-electron frictional force, $\mathbf{R}_i^{ie}$, and associated heat exchange terms, Q_i^{ie} and Q_e^{ie}, which appear in the three-component ion-electron-neutral model of Section III B. (Note that the ion-electron frictional force and heat exchange terms cancel when the two-component plasma-neutral model is formulated.) Purely Maxwellian reacting distribution functions (i.e., $f_\alpha = f_\alpha^0$) are assumed when taking moments of reaction collision operators. Thus, the non-Maxwellian effects due to thermal gradients in the CX friction terms $\mathbf{R}_{in}^{cx}$ and $\mathbf{R}_{in}^{cx}$ and associated thermal energy exchange terms are neglected in the present derivation.

Specific closures for each equation of the plasma-neutral model of Section III C are now discussed. The reaction-related terms, i.e., $\Gamma_\alpha^{react.}$, $\mathbf{R}_\alpha^{react.}$, and $Q_\alpha^{react.}$, do not technically fall into the "closure" category — non-Maxwellian effects are not included in those terms. However, discussion of their quantification is included below and relevant references are supplied.

Closure of continuity equations

To compute Γ_i^{ion} and Γ_n^{rec}, the ionization and recombination rate parameters arising in Eqns. (13) and (14) must be specified. For hydrogenic atoms, an approximation for the ionization rate parameter in terms of electron temperature (which may be assumed, e.g., to be equal to the ion temperature) is supplied by McWhirter [25]. As discussed by Meier [20], $\langle \sigma_{ion} v_e \rangle$ for the first 28 elements can be determined with the fitting formula and associated data given by Voronov [26]. An approximation for the radiative recombination rate parameter in terms of electron temperature is presented by McWhirter [25]. Goldston [27] provides a useful discussion of these rate parameters.

Closure of momentum equations

In Section III A, the resonant CX-related terms are defined, but the functional dependence of $\sigma_{cx}(V_{cx})$ on V_{cx} is not specified. An appropriate form for the hydrogenic CX cross-section, based on CX data from Barnett [28], is $\sigma_{cx,H} = 1.09 \times 10^{-18} - 7.15 \times 10^{-20} \ln(V_{cx})\ \mathrm{m}^2$. This formula matches the Barnett data to within 10% for relative ion-neutral particle speeds between

4.8×10^3 m/s and 1.4×10^6 m/s (i.e., between 0.12 eV and 10 keV for hydrogen).

The stress tensors Π and Π_n may be replaced with standard formulas. For example, assuming isotropic unmagnetized plasma viscosity and neglecting compressibility effects, $\Pi = -\xi[\nabla\mathbf{v} + (\nabla\mathbf{v})^\intercal]$, where ξ is the isotropic dynamic viscosity coefficient given by Braginskii [1]. Similarly, the neutral fluid stress tensor may be approximated as $\Pi_n = -\xi_n[\nabla\mathbf{v}_n + (\nabla\mathbf{v}_n)^\intercal]$. The neutral dynamic viscosity coefficient may be calculated using a rigid elastic sphere model as presented in Chapman and Cowling [18].

In many cases, the terms $\mathbf{R}_i^{in}$ and $\mathbf{R}_e^{en}$ are negligible. Goldston [27] shows that neutral-charged particle collisions are unimportant compared to Coulomb collisions for plasmas that are "even a few percent ionized". If the model is applied to a problem in which interesting physics occurs in regions of very low ionization, these terms should be addressed and included. Schunk and Nagy [29] propose treating neutral-charged particle interactions as Maxwell molecule collisions. See also the related astrophysical work of Leake et al. [30], in which the plasma-neutral model of Section III C is employed to simulate the weakly ionized solar chromosphere.

Closure of generalized Ohm's law

The electron-neutral scattering term $\mathbf{R}_e^{en}$ should be treated appropriately, as discussed in the previous section on the momentum equation closures. The terms $\mathbf{j} \times \mathbf{B}/(en)$ (the Hall term) and $\nabla \cdot \mathbb{P}_e/(en)$ (the diamagnetic term) may be retained if electron fluid effects are of interest. Several sources [1, 31, 32] provide detailed discussion of the range of validity for these assumptions. A particularly important requirement is that length scales of interest should be much larger than the ion gyroradius.

The frictional drag term, $-\mathbf{R}_i^{ie}/(en)$ is generally anisotropic with drag forces perpendicular to the magnetic field being a factor of two stronger than those parallel to the field. Braginskii [1] provides details for computing this drag term with anisotropic resistivity (e.g., $\hat{\eta} \cdot \mathbf{j}$, where $\hat{\eta}$ is a tensor resistivity) or with isotropic resistivity (e.g., $\eta\mathbf{j}$, where η is a scalar resistivity). In some cases, it may be appropriate to include anomalous effects in resistivity, e.g., Chodura resistivity; see the dissertation by Meier [20].

Closure of energy equations

Several reaction-related terms in the energy equations are as yet unspecified. The resonant CX-related terms in the energy equations are defined in Section III A. The resonant CX cross-section, $\sigma_{cx}(V_{cx})$, can be specified as discussed in the preceding discussion regarding closure of momentum equations. Formulas for Q_n^{ion} and Q_i^{rec} are defined in composing Eqns. (32) and (35), respectively. As discussed with regard to Eqn. (36), the conversion of electron thermal energy is defined as $Q_e^{rec} \equiv 1/2 m_e n_i \int f_e \sigma_{rec} w^3 d\mathbf{v}$. Parameterization of this integral in terms of T_e seems feasible, but Q_e^{rec} can be neglected if electron thermal energy loss in radiative recombination is not expected to play an important role in the energy balance. (Note that in formulating Eqn. (66), the electron kinetic energy transfer due to recombination is dropped in the $m_e \to 0$ limit. Because Q_e^{rec} involves thermal energy, however, it should be evaluated prior to applying the $m_e \to 0$ limit.)

The terms containing factors of $\mathbf{R}_i^{in}$ and $\mathbf{R}_e^{en}$ are neglected here for the same reasons that these charged-neutral friction forces are neglected in the momentum equations. The charged-neutral particle scattering terms, Q_i^{in} and Q_e^{en}, are dropped for the same reasons. The stress tensors, Π and Π_n, can be approximated as discussed for the momentum equations.

Under the assumption that scattering collisions dominate the species Boltzmann equations, heat flux closures can be taken from prior work, specifically Braginskii [1] (for the plasma heat flux), and Chapman and Cowling [18] (for the neutral heat flux). The plasma-neutral heat fluxes are

$$\mathbf{h} = -\left[\kappa_{\|}\hat{\mathbf{b}}\hat{\mathbf{b}} + \kappa_{\perp}\left(\mathbb{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}\right)\right] \cdot \nabla T - \frac{\gamma p_e \mathbf{j}}{n q_e (\gamma - 1)}, \tag{68}$$

and

$$\mathbf{h}_n = -\kappa_n \nabla T_n. \tag{69}$$

In the plasma heat flux, $\mathbf{h}$, the $\kappa_{\|}$ and $\kappa_{\perp}$ account for the effects of ion and electron thermal conductivity parallel and perpendicular, respectively, to the magnetic field direction which is given by the unit vector $\hat{\mathbf{b}} \equiv \mathbf{B}/|\mathbf{B}|$. The part of the plasma heat flux proportional to the electron pressure, p_e, accounts for the convection of electron thermal energy. In the neutral heat flux, $\mathbf{h}_n$, κ_n is the thermal conductivity. The conductivities $\kappa_{\|}$ and $\kappa_{\perp}$ are given by Braginskii [1]. The neutral heat flux is derived by Chapman and Cowling [18] using a rigid elastic sphere model.

If the CX collision frequency is higher than the neutral-neutral scattering frequency, it can be desirable to adopt a different closure for neutral heat flux. The form of the neutral thermal conductivity under the assumption of strong scattering is

$$\kappa_{n,hs} \propto \frac{n_n T_n}{\nu_{hs}}, \tag{70}$$

where ν_{hs} is the neutral-neutral scattering frequency, defined as $\nu_{hs} \equiv \bar{C}\pi d^2 n_n$, where $\bar{C}$ is the mean neutral velocity defined by $(\bar{C})^2 \equiv 8k_b T_n/(\pi m_n)$, and d is the diameter of a hard sphere representing the relevant atom. An alternative form is

$$\kappa_{n,cx-hs} \propto \frac{n_n T_n}{\nu_{cx-hs}}, \tag{71}$$

where $\nu_{cx-hs} \equiv \nu_{cx}+\nu_{hs}$. The CX frequency is defined as $\nu_{cx} \equiv \bar{C}n\sigma_{cx}$, where n is the plasma number density and σ_{cx} is the CX cross section. While this approximation is *ad hoc*, it approximates the perpendicular thermal transport intuitively expected in regions where CX competes with scattering to determine the neutral mean free path, such as, for example, the edge of a magnetically confined plasma. As discussed by Meier [20], when CX dominates scattering, the conductivity given by Eqn. (71) closely resembles the heat flux derived by Helander et al. [17].

IV. CONCLUSIONS

The derivation of Section III offers an extension of the derivations by Braginskii [1] of two-fluid and single-fluid plasma models to include a reacting neutral species. In Section III B, a reacting and interacting three-component electron-ion-neutral model is derived from Boltzmann equations with elastic scattering collisions and three inelastic reacting collisions: resonant charge exchange, electron-impact ionization, and radiative recombination. Moments of the reaction collision terms are described in detail. The three-component model is then reduced to a two-component plasma-neutral model in Section III C. Suggested closures are discussed for the plasma-neutral model in Section III D.

In future work, the plasma-neutral model could be extended to a general multi-fluid plasma model: multiple plasma and neutral species could be accommodated; multiply-charged ions could be allowed; excited states could be tracked; radiation effects could be included; as discussed in Section III D, the successive approximation technique employed to determine the local distribution functions could be generalized to more accurately close the plasma-neutral model; charged-neutral elastic collisions could be included, and should be included in problems where the ionization fraction is low; and additional reactions could be included such as non-resonant charge, three-body recombination, polarization ionization, etc. With so many possibilities, future model development efforts should target the extensions that are most important and useful for the anticipated applications.

V. ACKNOWLEDGMENTS

This work has been performed under the auspices of the U.S. Department of Energy by the University of Washington under Contract DE-FC02-05ER54811 and by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

[1] S. I. Braginskii, in *Rev. Plasma Phys., Vol. 1*, edited by M. A. Leontovitch (Consultants Bureau, New York, NY, 1965) pp. 205 – 311.

[2] G. P. Zank, Space Sci. Rev. **89**, 413 (1993).

[3] H. L. Pauls, G. P. Zank, and L. L. Williams, J. Geophys. Research **100**, 21,595 (1995).

[4] V. B. Baranov and Y. G. Malama, J. Geophys. Res. **98**, 15157 (1993).

[5] T. V. Zaqarashvili, M. L. Khodachenko, and H. O. Rucker, Astron. Astrophys. **529**, A82 (2011).

[6] T. D. Rognlien, J. L. Milovich, M. E. Rensink, and G. D. Porter, J. Nucl. Mater. **196**, 347 (1992).

[7] T. D. Rognlien, D. D. Ryutov, N. Mattor, and G. D. Porter, Phys. Plasmas **6**, 1851 (1999).

[8] T. D. Rognlien and M. E. Rensink, Fusion Eng. Design **60**, 497 (2002).

[9] R. Schneider, D. Reiter, H. P. Zehrfeld, B. Braams, M. Baelmans, J. Geiger, H. Kastelewicz, J. Neuhauser, and R. Wunderlich, J. Nucl. Mater. **196**, 810 (1992).

[10] R. Schneider, X. Bonnin, K. Borrass, D. P. Coster, H. Kastelewicz, D. Reiter, V. A. Rozhansky, and B. J. Braams, Contrib. Plasma Phys. **46**, 3 (2006).

[11] D. Stotler and C. Karney, Contrib. Plasma Phys. **34**, 392 (1994).

[12] D. Reiter, *The EIRENE code, Version Jan. 92, User manual* (www.eirene.de) KFS Jülich report JUEL-2599 (Mar. 1992).

[13] X. Q. Xu, R. H. Cohen, T. D. Rognlien, and J. R. Myra, Phys. Plasmas **7**, 1951 (2000).

[14] V. A. Izzo, D. G. Whyte, R. S. Granetz, P. B. Parks, E. M. Hollmann, L. L. Lao, and J. C. Wesley, Phys. Plasmas **15**, 056109 (2008).

[15] V. A. Izzo, P. B. Parks, and L. L. Lao, Plasma Phys. Contr. Fusion **51**, 105004 (2009).

[16] S. You, *Computational and Experimental Studies of Tokamak Refuelling*, Ph.D. thesis, Imperial College (2002).

[17] P. Helander, S. I. Krasheninnikov, and P. J. Catto, Phys. Plasmas **1**, 3174 (1994).

[18] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases* (Cambridge, 1970) third edition.

[19] H. W. Ripken and H. J. Fahr, Astron. and Astrophys. **122**, 181 (1983).

[20] E. T. Meier, *Modeling plasmas with strong anisotropy, neutral fluid effects, and open boundaries*, Ph.D. thesis, University of Washington (2011).

[21] U. Shumlak and J. Loverich, J. Comp. Phys. **187**, 620 (2003).

[22] U. Shumlak, R. Lilly, N. Reddell, E. Sousa, and B. Srinivasan, Comput. Phys. Commun. **182**, 1767 (2011).

[23] J. A. Bittencourt, *Fundamentals of Plasma Physics* (Permagon, 1986).

[24] M. Goosens, *An Introduction to Plasma Astrophysics and Magnetohydrodynamics* (Kluwer, 2003).

[25] R. W. P. McWhirter, in *Plasma Diagnostic Techniques*, edited by R. H. Huddlestone and S. L. Leonard (Academic Press, New York, 1965).

[26] G. S. Voronov, Atomic Data Nucl. Data **65**, 1 (1997).

[27] R. J. Goldston and P. H. Rutherford, *Introduction to Plasma Physics* (IOP Publishing Ltd., 1995).

[28] C. F. Barnett, *Atomic Data for Fusion, Vol. 1* (Oak Ridge National Laboratory, 1990).

[29] R. W. Schunk and R. W. Nagy, *Ionospheres* (Cambridge, 2000).

[30] J. E. Leake, M. G. Linton, and V. S. Lukin, Bulletin of the American Astronomical Society, Vol. 45, AAS Meeting # 220, 124.04.

[31] N. Krall and A. Trivelpiece, *Principles of Plasma Physics* (McGraw-Hill, 1973).

[32] J. P. Freidberg, Rev. Modern Phys. **54**, 801 (1982).

[33] A. H. Glasser and X. Z. Tang, Comput. Phys. Commun. **164**, 237 (2004).

[34] V. S. Lukin, *Computational Study of the Internal Kink Mode Evolution and Associated Magnetic Reconnection Phenomena*, Ph.D. thesis, Princeton University (2008).