

## Multicomponent, reacting MHD flows

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**Summary.** The equations describing multicomponent, reacting MHD flows are derived. Arbitrarily oriented magnetic fields are considered. The differential equations are obtained for: (1) general flows, and (2) the special case of plane-parallel, steady flows. The approximations made in deriving these equations are critically assessed. Particular attention is given to the momentum and energy ‘source terms’. Exact formulae are obtained for the momentum and energy source terms for elastic scattering for two special cases of the momentum transfer cross section: (1)  $\tilde{\sigma} \propto v^{-1}$ ; and (2)  $\tilde{\sigma} = \text{constant}$ . The effects of reactive processes, such as recombination, photoionization, photodissociation, charge exchange, and reactive scattering are also discussed. Departures from Maxwellian velocity distributions are considered.

### 1 Introduction

In recent years it has been recognized that the multifluid nature of MHD flows in interstellar clouds can be of great importance. Because the magnetic field interacts directly only with the ion-electron plasma, shock waves in clouds of low fractional ionization may contain extended regions in which the fluid velocities of the ions and neutrals differ appreciably, and this ion-neutral streaming can play a major role in momentum and energy transfer.

The equations describing steady, plane-parallel multifluid MHD flows were given by Draine (1980; hereafter D80) and Draine, Roberge & Dalgarno (1983; hereafter DRD83) for the special case where the magnetic field  $\vec{B}$  is transverse to the direction of shock propagation. These equations were used in numerical calculations of the shock wave believed to be responsible for the intense molecular line emission from OMC–1 (Draine & Roberge 1982; Chernoff, Hollenbach & McKee 1982), and in general studies of molecular line emission from a broad range of shock models (DRD83; Draine & Roberge 1984).

Flower, Pineau des Forets & Hartquist (1985; hereafter FPH85) have recently studied chemical reactions in steady, plane-parallel, transverse MHD shock waves in diffuse clouds. To compute

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the structure of these shock waves, FPH85 adopted equations of energy conservation for the electrons and ions differing from those of D80 and DRD83.

As it appears likely that study of MHD shock waves in molecular clouds will be of considerable and continuing interest, it is desirable to present a rigorous derivation of the equations describing such flows in order to clarify the disagreement between D80 and DRD83, on the one hand, and FPH85 on the other. At the same time, the MHD equations describing steady, plane-parallel flows will be extended to the general case where, in particular, the magnetic field  $\vec{B}$  is not required to be perpendicular to the direction of shock propagation. Finally, detailed consideration will be given to the ‘source terms’ in the MHD equations which describe the exchange of mass, momentum, and energy between the neutral, ion, and electron fluids.

In Section 2 we derive the equations expressing conservation of mass, momentum, and energy. In Section 3 we examine the ‘source terms’ associated with elastic scattering processes. In Section 4 the effects of chemical reactions are considered. Our results are compared with those of FPH85 in Section 5, where we also discuss the validity of various approximations adopted in deriving the MHD equations. Finally, our results are summarized in Section 6.

## 2 Conservation laws for multicomponent fluid flows

### 2.1 NOTATION AND ASSUMPTIONS

Consider a system of three interpenetrating fluids: neutrals, ions, and electrons, denoted by subscripts n, i, e. Fluid variables will be denoted by the subscript f, where  $f \in \{n, i, e\}$ . Each fluid will be characterized by the number density  $n_f$ , mass density  $\rho_f$ , flow velocity  $\vec{v}_f$ , temperature  $T_f$  [such that the mean translational kinetic energy per fluid particle in a frame moving with the fluid is  $(3/2)kT_f$ ], and internal energy per particle  $u_f$  (due to rotational, vibrational, or electronic excitation).

It is assumed that the neutral and ion fluids each consist of a number of distinct chemical species. The subscript  $\alpha$  will be used to denote a particular chemical species;  $n_\alpha$  and  $m_\alpha$  are the number density and molecular mass of that species, and  $n_f$  and  $\rho_f$  are given by

$$n_f = \sum_{\alpha \in f} n_\alpha, \quad (2.1)$$

$$\rho_f = \sum_{\alpha \in f} n_\alpha m_\alpha. \quad (2.2)$$

We will assume that the length scales for variation in the fluid variables  $n_f$ ,  $\rho_f$ ,  $\vec{v}_f$ , and  $T_f$  are long compared to the mean free path against scattering, so that a fluid description is meaningful. We will neglect viscous stresses; i.e., we will assume that the velocity distribution function for each fluid is locally isotropic in the frame of reference moving with the fluid. Particle diffusion\* and heat diffusion will be neglected. The validity of these and other assumptions will be discussed in Section 5.3.

The notion of a *comoving fluid element* is useful in formulating the conservation laws. The comoving fluid element has a (time-dependent) volume  $\Omega_f(t)$ , and the closed surface bounding this volume moves with the local fluid velocity  $\vec{v}_f$  (at the surface). In the limit  $\Omega_f \rightarrow 0$  one has

$$\frac{D_f \Omega_f}{Dt} = \Omega_f \nabla \cdot \vec{v}_f \quad (2.3)$$

where  $D_f/Dt \equiv \vec{v}_f \cdot \nabla + \partial/\partial t$  is the usual convective derivative for fluid f.

\* We assume that individual chemical species do not diffuse relative to other species belonging to the same fluid (e.g., He does not diffuse relative to H or H<sub>2</sub>). The neutrals and ions (and neutrals and electrons) are of course permitted to ‘diffuse’ through one another.

## 2.2 NUMBER CONSERVATION

The basic equation governing the rate of change of the number density  $n_\alpha$  of species  $\alpha$  belonging to fluid  $f$  is just (neglecting diffusion)

$$\frac{D_f}{Dt} (n_\alpha \Omega_f) = N_\alpha \Omega_f, \quad (2.4)$$

where  $N_\alpha$  is the net rate per volume at which species  $\alpha$  is being created by chemical reactions. Using equation (2.3) above, this gives the familiar result

$$\nabla \cdot (n_\alpha \vec{v}_f) + \frac{\partial n_\alpha}{\partial t} = N_\alpha. \quad (2.5)$$

## 2.3 MASS CONSERVATION

The fundamental equation of mass conservation (neglecting diffusion) is

$$\frac{D_f}{Dt} (\rho_f \Omega_f) = S_f \Omega_f, \quad (2.6)$$

where  $S_f$  is the rate per volume at which mass is being added to fluid  $f$  by chemical reactions. Using (2.3) one obtains

$$\nabla \cdot (\rho_f \vec{v}_f) + \frac{\partial \rho_f}{\partial t} = S_f. \quad (2.7)$$

## 2.4 MOMENTUM CONSERVATION

The momentum  $\rho_n \Omega_n \vec{v}_n$  of the neutral fluid within the comoving fluid element  $\Omega_n$  can be changed only by (i) the pressure exerted by the neutral fluid on the boundaries of the fluid element; (ii) the gravitational force; (iii) non-reactive scattering with particles of other fluids; (iv) creation or destruction of neutral particles by 'chemical' processes. The fundamental equation of momentum conservation is

$$\frac{D_n}{Dt} (\rho_n \Omega_n \vec{v}_n) = -\Omega_n \nabla (n_n k T_n) - \rho_n \Omega_n \nabla \Phi + \vec{F}_n \Omega_n, \quad (2.8)$$

where  $\Phi$  is the gravitational potential, and  $\vec{F}_f$  is the rate at which the momentum per volume of fluid  $f$  is changed as the result of non-reactive scatterings as well as chemical processes. The fundamental equation for momentum conservation of the neutrals is then

$$\frac{D_n}{Dt} (\rho_n \vec{v}_n) + \rho_n \vec{v}_n \nabla \cdot \vec{v}_n + \nabla (n_n k T_n) = \vec{F}_n - \rho_n \nabla \Phi. \quad (2.9a)$$

For the special case of plane-parallel, stationary flows ( $\partial/\partial x = \partial/\partial y = \partial/\partial t = 0$ ) this simplifies to

$$\frac{d}{dz} (\rho_n \vec{v}_n v_{nz} + n_n k T_n \hat{e}_z) = \vec{F}_n - \rho_n \nabla \Phi, \quad (2.9b)$$

where  $\hat{e}_z$  is the unit vector in the  $z$  direction. We assume that the charged particles (ions and electrons) all have a common fluid velocity  $\vec{v}_i$ , since differences in the *divergence* of the ion and electron velocities would lead to charge separation and strong electric fields opposing this charge

separation. While differences in the fluid velocities of the ions and electrons (i.e., electric currents) are of course required if magnetic field gradients exist, it will be seen below (Section 5.3) that the drift velocities associated with these currents are negligible compared to the fluid velocities for all cases of interest. Since it is assumed that no net charge density is present, it follows that there is no change of momentum due to the electric field  $\vec{E}$ . Writing down a fundamental equation of momentum conservation for the ions and electrons which is similar to equation (2.8), but with an added term  $\Omega_i \vec{J} \times \vec{B}/c$  on the right-hand side representing the Lorentz force on the fluid element, we obtain {using  $\nabla \times \vec{B} = (4\pi/c)\vec{J} + (1/c)\partial\vec{D}/\partial t$ }

$$\frac{D_i}{Dt} (\rho_i \vec{v}_i) + \rho_i \vec{v}_i \nabla \cdot \vec{v}_i + \nabla \left( n_i k T_i + n_e k T_e + \frac{B^2}{8\pi} \right) - \frac{1}{4\pi} (\vec{B} \cdot \nabla) \vec{B} + \frac{1}{4\pi c} \frac{\partial \vec{D}}{\partial t} \times \vec{B} = \vec{F}_i + \vec{F}_e - \rho_i \nabla \Phi. \quad (2.10a)$$

For the special case of plane-parallel steady flows this simplifies to

$$\frac{d}{dz} \left\{ \rho_i \vec{v}_i v_{iz} + \hat{e}_z \left( n_i k T_i + n_e k T_e + \frac{B^2}{8\pi} \right) \right\} - \frac{1}{4\pi} B_z \frac{\partial}{\partial z} \vec{B} = \vec{F}_i + \vec{F}_e - \rho_i \nabla \Phi. \quad (2.10b)$$

It is worth noting that the derivation of (2.10a) and (2.10b) did not rely on any assumption regarding the conductivity of the plasma (except in so far as the ion and electron velocities were taken to be equal).

## 2.5 ELECTRODYNAMICS

We assume the plasma to be a perfect electrical conductor, so that the electric field vanishes in the frame comoving with the plasma. Thus in a general frame we have  $\vec{E} = -\vec{v}_i \times \vec{B}/c$ . Operating with  $\nabla \times$  and using the Maxwell equation  $\nabla \times \vec{E} = -\partial \vec{B}/\partial t$ , we obtain

$$\frac{\partial \vec{B}}{\partial t} = \nabla \times (\vec{v}_i \times \vec{B}). \quad (2.11)$$

For the special case of plane-parallel, steady flow we obtain

$$\frac{d}{dz} (\vec{B} v_z) = B_z \frac{d}{dz} \vec{v}_i, \quad (2.12)$$

from which we obtain (using  $\nabla \cdot \vec{B} = 0$ )

$$B_z = \text{constant}, \quad (2.13a)$$

$$\frac{d}{dz} (B_x v_{iz}) = B_z \frac{d}{dz} v_{ix}, \quad (2.13b)$$

$$\frac{d}{dz} (B_y v_{iz}) = B_z \frac{d}{dz} v_{iy}. \quad (2.13c)$$

## 2.6 ENERGY CONSERVATION

The ‘thermal’ energy content of the fluid element  $\Omega_f$  consists of the kinetic energy  $(3/2)n_f \Omega_f k T_f$  in random motions of the particles, plus  $n_f \Omega_f u_f$ , where  $u_f$  is the mean internal energy per particle due to excitation of internal degrees of freedom (rotation, vibration, etc.). The fundamental

equation for the rate of change of the thermal energy content of the fluid element is

$$\frac{D_f}{Dt} \left\{ n_f \Omega_f \left( \frac{3}{2} k T_f + u_f \right) \right\} = -n_f k T_f \frac{D_f \Omega_f}{Dt} + G_f \Omega_f, \quad (2.14)$$

where  $G_f$  is the rate of change per volume of the thermal energy content of fluid  $f$  due to interaction with other fluids, emission or absorption of radiation, interaction with cosmic rays, etc. The term on the right-hand side involving  $D_f \Omega_f / Dt$  is just the change in thermal energy of the fluid associated with adiabatic compression or expansion of the fluid element. Heat diffusion (i.e., thermal conduction) has been neglected. It is important to note that equation (2.14) applies to the electron and ion fluids as well as to the neutral particles.\* Equation (2.14) may be rewritten

$$\frac{D_f}{Dt} \left\{ n_f \left( \frac{3}{2} k T_f + u_f \right) \right\} + \left\{ n_f \left( \frac{5}{2} k T_f + u_f \right) \right\} \nabla \cdot \vec{v}_f = G_f. \quad (2.15a)$$

For the special case of plane-parallel, steady flow this becomes

$$\frac{d}{dz} \left\{ n_f \left( \frac{3}{2} k T_f + u_f \right) v_{fz} \right\} + n_f k T_f \frac{d}{dz} v_{fz} = G_f. \quad (2.15b)$$

An alternative energy conservation equation for plane-parallel, steady flow is sometimes useful. To obtain this equation for the neutral fluid, operate on equation (2.9b) with  $v_{nz} \hat{e}_z$ , add the result to (2.15b), and use (2.7) to obtain

$$\frac{d}{dz} \left\{ \frac{1}{2} \rho_n v_{nz}^3 + n_n v_{nz} \left( \frac{5}{2} k T_n + u_n \right) \right\} = G_n + F_{nz} v_{nz} - \frac{1}{2} S_n v_{nz}^2 - \rho_n v_{nz} \frac{d\Phi}{dz}. \quad (2.16)$$

For the ion-electron plasma, operate on equation (2.10b) with  $v_{iz} \hat{e}_z$ , add the result to (2.15b) for the ions plus electrons, and use (2.7) and (2.13) to obtain

$$\begin{aligned} & \frac{d}{dz} \left[ \frac{1}{2} \rho_i v_{iz}^3 + v_{iz} \left\{ \frac{5}{2} (n_i k T_i + n_e k T_e) + \frac{1}{4\pi} (B_x^2 + B_y^2) \right\} \right] \\ &= G_i + G_e + (F_{iz} + F_{ez}) v_{iz} - \frac{1}{2} S_i v_{iz}^2 + \frac{B_z}{4\pi} \left( B_x \frac{dv_x}{dz} + B_y \frac{dv_y}{dz} \right) - \rho_i v_{iz} \frac{d\Phi}{dz}. \end{aligned} \quad (2.17)$$

### 3 Source terms: elastic scattering

$N_f$ ,  $S_f$ ,  $\vec{F}_f$ , and  $G_f$  – the source terms for particle number, mass, momentum, and thermal energy – have the same definitions here as in previous work by D80 and DRD83. In those papers expressions were given for the contributions to these source terms due to a few selected processes, such as ion-neutral elastic scattering, ion-electron elastic scattering, etc. A more comprehensive discussion of these terms is provided below.

#### 3.1 GENERAL RESULTS

We consider species  $\alpha$  and  $\beta$ , each assumed to have a Maxwellian velocity distribution (with temperatures  $T_\alpha$  and  $T_\beta$ , respectively) centred around mean velocities  $\vec{v}_\alpha$  and  $\vec{v}_\beta$ . Let  $d\sigma(v, \theta)/d\Omega$  be the differential cross-section for elastic scattering, where  $v$  is the relative velocity of the collision partners, and  $\theta$  is the deflection angle in the centre-of-mass frame. Then

\* Ohmic heating, though usually negligible (see Section 5.3 below) would enter as a contribution to  $G_f$ , as it is the direct result of scattering of the current carriers by other species.

the general expression for the contribution of elastic scattering to the momentum source term  $\vec{F}$  for species  $\alpha$  is (see Appendix A):

$$\vec{F}_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})} \left( \frac{2kT_r}{\pi m_r} \right)^{1/2} (\vec{v}_{\beta} - \vec{v}_{\alpha}) \times s^{-3} \exp(-s^2) \int_0^{\infty} dx x^2 \tilde{\sigma}(v = xc_r) \exp(-x^2) \{2xs \cosh(2xs) - \sinh(2xs)\}, \quad (3.1)$$

where

$$m_r \equiv \frac{m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})} \quad (3.2)$$

$$T_r \equiv \frac{m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha}}{(m_{\alpha} + m_{\beta})} \quad (3.3)$$

$$s \equiv \frac{|\vec{v}_{\alpha} - \vec{v}_{\beta}|}{c_r} \quad (3.4)$$

$$c_r \equiv \left( \frac{2kT_r}{m_r} \right)^{1/2} \quad (3.5)$$

and

$$\tilde{\sigma}(v) \equiv \int d\Omega \frac{d\sigma}{d\Omega} (1 - \cos \theta) \quad (3.6)$$

is the momentum-transfer cross-section for elastic scattering.

The general expression for the contribution of elastic scattering to the heat source term  $G$  for species  $\alpha$  is (see Appendix B):

$$G_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})^2} \left( \frac{8kT_r}{\pi m_r} \right)^{1/2} \exp(-s^2) 2k \times \left\{ \left( \frac{T_{\beta} - T_{\alpha}}{s} \right) \times \int_0^{\infty} dx x^4 \tilde{\sigma}(v = xc_r) \exp(-x^2) \sinh(2xs) + \frac{m_{\beta} T_{\alpha}}{m_r} \times \int_0^{\infty} dx x^3 \tilde{\sigma}(v = xc_r) \exp(-x^2) \cosh(2xs) - \frac{m_{\beta} T_{\alpha}}{2m_r s} \times \int_0^{\infty} dx x^2 \tilde{\sigma}(v = xc_r) \exp(-x^2) \sinh(2xs) \right\}. \quad (3.7)$$

### 3.2 SPECIAL CASE: $\tilde{\sigma}v = \text{CONSTANT}$

A special case of particular interest is that where the momentum transfer cross-section  $\tilde{\sigma} \propto v^{-1}$ , since this applies to scattering by an  $r^{-4}$  potential, a good approximation to the polarization interaction between ions and neutral atoms or molecules. For this case the integrals in (3.1) and (3.7) simplify greatly, with the result

$$\vec{F}_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})} (\tilde{\sigma}v) (\vec{v}_{\beta} - \vec{v}_{\alpha}) \quad (3.8)$$

$$G_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})^2} (\tilde{\sigma}v) \{3k(T_{\beta} - T_{\alpha}) + m_{\beta} |\vec{v}_{\alpha} - \vec{v}_{\beta}|^2\}. \quad (3.9)$$

### 3.3 SPECIAL CASE: $\tilde{\sigma} = \text{CONSTANT}$

A second case of interest is that of elastic scattering by a velocity-independent cross-section. For this case one obtains

$$\vec{F}_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})} \left( \frac{2kT_r}{\pi m_r} \right)^{1/2} (\vec{v}_{\beta} - \vec{v}_{\alpha}) I_1(s) \quad (3.10)$$

$$I_1 \equiv \left( 1 + \frac{1}{2s^2} \right) \exp(-s^2) + \left( s + \frac{1}{s} - \frac{1}{4s^3} \right) \pi^{1/2} \text{erf}(s). \quad (3.11)$$

An excellent approximation to  $I_1$  is provided by

$$I_1 \approx \frac{8}{3} \left( 1 + \frac{9\pi s^2}{64} \right)^{1/2} \quad (3.12)$$

which is exact in the limits  $s \rightarrow 0$  and  $s \rightarrow \infty$ , and is accurate to within 1.5 per cent for  $0 < s < \infty$ . The heat source term is

$$G_{\alpha, \text{elas. scat.}} = \frac{n_{\alpha} n_{\beta} m_{\alpha} m_{\beta}}{(m_{\alpha} + m_{\beta})^2} \left( \frac{8kT_r}{\pi m_r} \right)^{1/2} \tilde{\sigma} k \left\{ (T_{\beta} - T_{\alpha}) I_2(s) + \left( \frac{m_{\alpha} + m_{\beta}}{m_{\alpha}} \right) T_{\alpha} I_3(s) \right\} \quad (3.13)$$

$$I_2 \equiv \left( s^2 + \frac{5}{2} \right) \exp(-s^2) + \left( \frac{3}{4s} + 3s + s^3 \right) \pi^{1/2} \text{erf}(s) \quad (3.14)$$

$$I_3 \equiv \left( s^2 + \frac{1}{2} \right) \exp(-s^2) + \left( s^3 + s - \frac{1}{4s} \right) \pi^{1/2} \text{erf}(s). \quad (3.15)$$

$I_2$  and  $I_3$  may be approximated by

$$I_2 \approx \left( 1 + \frac{9\pi s^2}{64} \right)^{1/2} \left( 4 + \frac{8}{3} s^2 \right), \quad (3.16)$$

(accurate to within 5.0 per cent for  $0 < s < \infty$ ), and

$$I_3 \approx \left( 1 + \frac{9\pi s^2}{64} \right)^{1/2} \frac{8}{3} s^2, \quad (3.17)$$

(accurate to within 1.5 per cent for  $0 < s < \infty$ ).

## 4 Source terms: chemical reactions

### 4.1 GENERAL FORMULAE

Let  $N_{\alpha, \lambda}$  be the rate per volume at which particles  $\alpha$  are being created (if  $N_{\alpha, \lambda} > 0$ ) or destroyed (if  $N_{\alpha, \lambda} < 0$ ) by a specific chemical reaction  $\lambda$ . By ‘chemical reaction’ we mean any process which creates or destroys particles of a particular species – i.e., we consider photoionization, photodissociation, electron–ion recombination, and charge exchange to be ‘chemical’ reactions.

In addition to the mean velocity  $\vec{v}_{\alpha}$  of species  $\alpha$ , we define the velocity  $\vec{w}_{\alpha, \lambda}$  to be the mean velocity of particles  $\alpha$  emerging from reaction  $\lambda$  (if the reaction is one which creates species  $\alpha$  – i.e.,  $N_{\alpha, \lambda} > 0$ ) or being destroyed by reaction  $\lambda$  (if the reaction is one which destroys species  $\alpha$  – i.e.,  $N_{\alpha, \lambda} < 0$ ). We also define  $\gamma_{\alpha, \lambda}$  to be the three-dimensional velocity dispersion of particles  $\alpha$  emerging from reaction  $\lambda$  (if  $N_{\alpha, \lambda} > 0$ ) or being destroyed by reaction  $\lambda$  (if  $N_{\alpha, \lambda} < 0$ ). With these



definitions, it is now straightforward to write down the rate per volume of creation of mass for species  $\alpha$ :

$$S_{\alpha,\lambda} = N_{\alpha,\lambda} m_{\alpha}; \quad (4.1)$$

the rate per volume of addition of momentum to species  $\alpha$  by reaction  $\lambda$ :

$$\vec{F}_{\alpha,\lambda} = N_{\alpha,\lambda} m_{\alpha} \vec{w}_{\alpha,\lambda}; \quad (4.2)$$

and the rate per volume of addition of thermal energy to species  $\alpha$  by reaction  $\lambda$ :

$$G_{\alpha,\lambda} = N_{\alpha,\lambda} (1/2 m_{\alpha} |\vec{v}_{\alpha} - \vec{w}_{\alpha,\lambda}|^2 + 1/2 m_{\alpha} \gamma_{\alpha,\lambda}^2). \quad (4.3)$$

The total source terms for fluid  $f$  are obtained by summing over all reactions  $\lambda$  involving components of  $f$ :

$$X_f = \sum_{\alpha \in f} \sum_{\lambda} X_{\alpha,\lambda} \quad (X = N, S, \vec{F}, \text{ or } G). \quad (4.4)$$

#### 4.2 ION-ELECTRON RADIATIVE RECOMBINATION

For radiative recombination  $\lambda = I^+ + e^- \rightarrow A + h\nu$  with rate coefficient  $\alpha$  we have

$$N_{A,\lambda} = -N_{I,\lambda} = -N_{e,\lambda} = \alpha n_I n_e \quad (4.5)$$

$$S_{A,\lambda} = -S_{I,\lambda} = \alpha n_I n_e m_A, \quad S_{e,\lambda} = -\alpha n_I n_e m_e \quad (4.6)$$

$$\vec{F}_{A,\lambda} = -\vec{F}_{I,\lambda} = \alpha n_I n_e m_A \vec{v}_i, \quad \vec{F}_{e,\lambda} = -\alpha n_I n_e m_e \vec{v}_i, \quad (4.7)$$

$$G_{A,\lambda} = \alpha n_I n_e (1/2 m_A |\vec{v}_n - \vec{v}_i|^2 + 3/2 k T_i), \quad (4.8)$$

$$G_{I,\lambda} = -\alpha n_I n_e 3/2 k T_i, \quad G_{e,\lambda} = -\alpha n_I n_e k T_e, \quad (4.9)$$

where we have assumed that: (i)  $T_e/m_e \gg T_i/m_I$  (so that the recombination rate is independent of the random velocity of a given ion); (ii)  $m_I \gg m_e$  (so that  $m_I \approx m_A$ , and the velocity of a newly-formed atom is equal to that of the ion which recombined to form it); (iii)  $\vec{v}_i = \vec{v}_e$ ; (iv) the radiative recombination cross-sections  $\sigma(v) \propto v^{-2}$ , so that the mean kinetic energy  $(1/2)m_e \gamma_{e, \text{rad. rec.}}^2$  of the recombining electrons is just  $kT_e$ .

#### 4.3 ION-ELECTRON DISSOCIATIVE RECOMBINATION

For exothermic dissociative recombination  $\lambda = I^+ + e^- \rightarrow A + B + \Delta E$  (where  $\Delta E > 0$  is the kinetic energy of the products minus the kinetic energy of the reactants) with rate coefficient  $\alpha$  we have

$$N_{A,\lambda} = N_{B,\lambda} = -N_{I,\lambda} = -N_{e,\lambda} = \alpha n_I n_e, \quad (4.10)$$

$$S_{A,\lambda} + S_{B,\lambda} = -S_{I,\lambda} = \alpha n_I n_e m_I, \quad S_{e,\lambda} = -\alpha n_I n_e m_e, \quad (4.11)$$

$$\vec{F}_{A,\lambda} + \vec{F}_{B,\lambda} = -\vec{F}_{I,\lambda} = \alpha n_I n_e m_I \vec{v}_i, \quad \vec{F}_{e,\lambda} = -\alpha n_I n_e m_e \vec{v}_i, \quad (4.12)$$

$$G_{A,\lambda} + G_{B,\lambda} = \alpha n_I n_e (1/2 m_I |\vec{v}_n - \vec{v}_i|^2 + 3/2 k T_i + k T_e + \Delta E), \quad (4.13)$$

$$G_{I,\lambda} = -\alpha n_I n_e 3/2 k T_i, \quad G_{e,\lambda} = -\alpha n_I n_e k T_e, \quad (4.14)$$

where we have made the same assumptions [(i)–(iv)] as in the preceding discussion of radiative recombination.



#### 4.4 PHOTOIONIZATION

For photoionization of a neutral  $\lambda = A + h\nu \rightarrow I^+ + e^- + \Delta E$  at a rate per volume  $n_A \xi_\lambda$  one has

$$N_{I,\lambda} = N_{e,\lambda} = -N_{A,\lambda} = n_A \xi_\lambda \quad (4.15)$$

$$S_{I,\lambda} = -S_{A,\lambda} = n_A \xi_\lambda m_A, \quad S_{e,\lambda} = n_A \xi_\lambda m_e \quad (4.16)$$

$$\vec{F}_{I,\lambda} = -\vec{F}_{A,\lambda} = n_A \xi_\lambda m_A \vec{v}_n, \quad \vec{F}_{e,\lambda} = n_A \xi_\lambda m_e \vec{v}_n, \quad (4.17)$$

$$G_{A,\lambda} = -n_A \xi_\lambda \frac{3kT_n}{2}, \quad (4.18)$$

$$G_{I,\lambda} = n_A \xi_\lambda (\frac{1}{2} m_I |\vec{v}_n - \vec{v}_i|^2 + \frac{3}{2} kT_n), \quad G_{e,\lambda} = n_A \xi_\lambda \Delta E. \quad (4.19)$$

#### 4.5 PHOTODISSOCIATION

Consider photodissociation  $\lambda = AB + h\nu \rightarrow A + B + \Delta E$ , where  $A$  and  $B$  are both neutral. Then

$$N_{A,\lambda} = N_{B,\lambda} = -N_{AB,\lambda} = n_{AB} \xi_\lambda, \quad (4.20)$$

$$S_{A,\lambda} + S_{B,\lambda} + S_{AB,\lambda} = 0, \quad (4.21)$$

$$\vec{F}_{A,\lambda} + \vec{F}_{B,\lambda} + \vec{F}_{AB,\lambda} = 0, \quad (4.22)$$

$$G_{A,\lambda} + G_{B,\lambda} + G_{AB,\lambda} = n_{AB} \xi_\lambda \Delta E. \quad (4.23)$$

If an ion is photodissociated into a neutral and an ion,  $\lambda = AI^+ + h\nu \rightarrow A + I^+ + \Delta E$ , then

$$N_{A,\lambda} = N_{I,\lambda} = -N_{AI,\lambda} = n_{AI} \xi_\lambda, \quad (4.24)$$

$$S_{A,\lambda} = -(S_{I,\lambda} + S_{AI,\lambda}) = n_{AI} \xi_\lambda m_A, \quad (4.25)$$

$$\vec{F}_{A,\lambda} = -(\vec{F}_{I,\lambda} + \vec{F}_{AI,\lambda}) = n_{AI} \xi_\lambda m_A \vec{v}_i, \quad (4.26)$$

$$G_{A,\lambda} = n_{AI} \xi_\lambda \left\{ \frac{1}{2} m_A |\vec{v}_n - \vec{v}_i|^2 + \frac{3m_A}{2(m_A + m_I)} kT_i + \frac{m_I \Delta E}{(m_A + m_I)} \right\}, \quad (4.27)$$

$$G_{I,\lambda} + G_{AI,\lambda} = n_{AI} \xi_\lambda \left\{ -\frac{3m_A}{2(m_A + m_I)} kT_i + \frac{m_A \Delta E}{(m_A + m_I)} \right\}. \quad (4.28)$$

#### 4.6 ION-MOLECULE REACTIONS WITH $k(T) = \text{CONSTANT}$

If the rate coefficient  $k_\lambda$  for an ion-molecule exchange reaction  $\lambda = A + I^+ \rightarrow B + J^+ + \Delta E$  is temperature independent (the reaction must be exothermic for this to be true), then the probability per time of a given particle  $A$  or  $I^+$  reacting is independent of its velocity, and we find

$$N_{B,\lambda} = N_{J,\lambda} = -N_{A,\lambda} = -N_{I,\lambda} = k_\lambda n_A n_I, \quad (4.29)$$

$$S_{A,\lambda} + S_{B,\lambda} = -(S_{I,\lambda} + S_{J,\lambda}) = k_\lambda n_A n_I (m_B - m_A). \quad (4.30)$$

We now assume no forward-backward asymmetry to the differential-scattering cross-section  $d\sigma(\theta, v)/d\Omega$  describing the reaction, i.e.,

$$\int (d\sigma/d\Omega) \cos \theta d\Omega = 0,$$

where  $\theta$  is the angle between the (incoming) velocity of  $A$  and the (outgoing) velocity of  $B$  in the centre-of-mass frame. This assumption is reasonable if the reaction proceeds via formation of a

long-lived 'intermediate complex'  $AI^+$  which loses 'memory' of the incoming directions of the reactants. With this assumption the mean velocity of the reaction products is zero in the centre-of-mass frame, and

$$\mathbf{F}_{A,\lambda} + \mathbf{F}_{B,\lambda} = -(\mathbf{F}_{I,\lambda} + \mathbf{F}_{J,\lambda}) = k_\lambda n_A n_I \left\{ \frac{m_A(m_B - m_A - m_I)\vec{v}_n}{(m_A + m_I)} + \frac{m_B m_I \vec{v}_i}{(m_A + m_I)} \right\}, \quad (4.31)$$

$$G_{I,\lambda} + G_{J,\lambda} = k_\lambda n_A n_I \left\{ \frac{m_A(m_A m_J + m_B m_I)}{2(m_A + m_I)^2} |\vec{v}_i - \vec{v}_n|^2 + \frac{m_B \Delta E}{m_A + m_I} + \frac{3k(m_A m_J + m_B m_I)}{2(m_A + m_I)^2} (T_n - T_i) \right\}, \quad (4.32)$$

$$G_{A,\lambda} + G_{B,\lambda} = k_\lambda n_A n_I \left\{ \frac{m_I(m_A m_J + m_B m_I)}{2(m_A + m_I)^2} |\vec{v}_i - \vec{v}_n|^2 + \frac{m_J \Delta E}{m_A + m_I} + \frac{3k(m_A m_J + m_B m_I)}{2(m_A + m_I)^2} (T_i - T_n) \right\}. \quad (4.33)$$

#### 4.7 OTHER ION-MOLECULE REACTIONS

If the cross-section  $\sigma(v)$  for a reaction  $\lambda = A + I^+ \rightarrow B + J^+ + \Delta E$  does not vary as  $v^{-1}$  (as must, for example, be true of endothermic reactions with  $\Delta E < 0$ ) then the effective rate coefficient for  $\lambda$  is given by (Draine & Katz 1986)

$$k_\lambda = \left( \frac{8kT_r}{\pi m_r s^2} \right)^{1/2} \int_0^\infty dx x^2 \sigma_\lambda(v = xc_r) \sinh(2xs) \exp\{-(x^2 + s^2)\}, \quad (4.34)$$

where  $T_r$ ,  $m_r$ ,  $c_r$ , and  $s$  are defined in equations (3.2–3.5). With this expression for  $k_\lambda$ , the number and mass source terms are given by equations (4.29) and (4.30). Calculating the momentum and heat source terms  $\vec{F}$  and  $G$  associated with such a reaction is complex, however, since  $\vec{F}$  and  $G$  depend upon the precise velocity dependence of the reaction cross-section  $\sigma(v)$  (the reaction will preferentially deplete particular parts of the reactant velocity distributions). Lacking detailed estimates for  $\vec{F}$  and  $G$ , however, a reasonable approximation is to use equations (4.31–4.33).

#### 4.8 CHARGE EXCHANGE $A + B^+ \rightarrow A^+ + B + \Delta E$

At low velocities charge exchange, if 'rapid', occurs via formation of an 'excited complex'  $AB^+$ , with a 'Langevin' rate coefficient  $k_\lambda \approx 10^{-9} \text{ cm}^3 \text{ s}^{-1}$  independent of temperature and drift velocity. In this low-velocity regime it is probably a good approximation to assume that there is no net forward-backward asymmetry to the scattering process, in which case the results of Section 4.6 (equations 4.29–4.33) are directly applicable with the substitutions  $I^+ \rightarrow B^+$ ,  $J^+ \rightarrow A^+$ :

$$\mathbf{F}_{A,\lambda} + \mathbf{F}_{B,\lambda} = -(\mathbf{F}_{A^+,\lambda} + \mathbf{F}_{B^+,\lambda}) = k_\lambda n_A n_{B^+} \frac{m_B^2 \vec{v}_i - m_A^2 \vec{v}_n}{m_A + m_B}, \quad (4.35)$$

$$G_{A,\lambda} + G_{B,\lambda} = k_\lambda n_A n_{B^+} \left\{ \frac{(m_A^2 + m_B^2)}{(m_A + m_B)^2} \left( \frac{1}{2} m_B |\vec{v}_i - \vec{v}_n|^2 + \frac{3}{2} k(T_i - T_n) \right) + \frac{m_A \Delta E}{m_A + m_B} \right\} \quad (4.36)$$

$$G_{A^+,\lambda} + G_{B^+,\lambda} = k_\lambda n_A n_{B^+} \left\{ \frac{(m_A^2 + m_B^2)}{(m_A + m_B)^2} \left( \frac{1}{2} m_A |\vec{v}_i - \vec{v}_n|^2 + \frac{3}{2} k(T_n - T_i) \right) + \frac{m_B \Delta E}{m_A + m_B} \right\}. \quad (4.37)$$

At higher velocities, the rate coefficient begins to increase with increasing velocity. In the high-velocity regime, the nuclei typically undergo very little deflection; in the limit of zero nuclear deflection one has

$$\vec{F}_{A,\lambda} + \vec{F}_{B,\lambda} = -(\vec{F}_{A^+,\lambda} + \vec{F}_{B^+,\lambda}) = k_\lambda n_A n_{B^+} (m_B \vec{v}_i - m_A \vec{v}_n), \quad (4.38)$$

$$G_{A,\lambda} + G_{B,\lambda} = \frac{1}{2} m_B |\vec{v}_i - \vec{v}_n|^2 + \frac{3}{2} k (T_i - T_n), \quad (4.39)$$

$$G_{A^+,\lambda} + G_{B^+,\lambda} = \frac{1}{2} m_A |\vec{v}_i - \vec{v}_n|^2 + \frac{3}{2} k (T_n - T_i). \quad (4.40)$$

In equations (4.38–4.40) we have neglected (as in Section 4.7 above) the fact that a velocity-dependent rate coefficient will lead to non-uniform depletion of the velocity distributions of  $A$  and  $B^+$ .

## 5 Discussion

FPH85 have recently discussed the effects of chemical reactions in MHD shocks. Their treatment of the dynamics of chemically-reacting multicomponent MHD flows differs from the present one in several respects. FPH85 adopted energy equations for the ions and electrons in these flows which differ from the equations of D80, DRD83, and the present paper. FPH85 have also presented results for the ‘source terms’ associated with chemical reactions in these flows which differ somewhat from those found here. These disagreements are discussed in Sections 5.1 and 5.2 below. Section 5.3 is devoted to consideration of the validity of the approximations used in deriving the MHD equations.

### 5.1 MHD EQUATIONS

FPH85 have discussed steady, plane-parallel, multicomponent MHD flows for  $B_z=0$ ,  $\mathbf{v}_f = v_{fz} \hat{z}$ , and  $\nabla\Phi=0$ . They have put forward the following equations (equations 12 and 13 of FPH85):

$$\frac{d}{dz} \left( \frac{1}{2} \rho_i v_i^3 + \frac{5}{2} n_i v_i k T_i + v_i \frac{B^2}{4\pi} \right) = B_i$$

$$\frac{d}{dz} \left\{ \frac{1}{2} \rho_i v_i^3 + \frac{5}{2} v_i (n_i k T_i + n_e k T_e) + v_i \frac{B^2}{4\pi} \right\} = B_i + B_e$$

where  $B_i$  and  $B_e$  on the right-hand-side are ‘source’ terms which presumably vanish in the absence of ion–electron, ion–neutral, or electron–neutral scattering, or chemical processes involving ions or electrons. Subtracting the first of these equations from the second one obtains

$$\frac{d}{dz} \left( \frac{5}{2} n_e v_i k T_e \right) = B_e.$$

This equation, if correct, would imply that in a flow with no ionization or recombination [so  $d(n_e v_i)/dz=0$ ] and no electron–ion or electron–neutral scattering (so  $B_e=0$ ) one would have  $T_e=\text{constant}$ . It is clear, however, that acceleration or deceleration of the electron–ion plasma must result in expansion or compression of the electrons, and that this expansion or compression will result in adiabatic cooling or heating of the electrons, as described by equation (2.15b) with  $G_e=0$ . It is also clear that such acceleration or deceleration of the electron–ion plasma can (in principle) take place even with no scattering of the electrons (i.e.,  $B_e=0$ ) as the result of ion–neutral scattering, a gradient in the magnetic pressure, or heating or cooling of the ions. If

the identification  $B_i + B_e = G_i + G_e + (F_{iz} + F_{ez})v_{iz} - (1/2)S_i v_{iz}^2$  is made, then equation (13) of FPH85 is in agreement with our equation (2.17). Equation (12) of FPH85 is therefore incorrect. \*

## 5.2 SOURCE TERMS

FPH85 have discussed the source terms associated with various chemical processes in multicomponent MHD flows, and have presented some general expressions for the heating effects of chemical reactions (equations 25–29 of FPH85) which differ from our results. As one simple example, we consider the contribution of electron–ion recombination to heating of the neutral fluid. FPH85 have adopted a notation which differs from that in this and previous papers (D80, DRD83); in particular, FPH85 have used the symbols  $B_n$ ,  $B_i$ , and  $B_e$  to denote total (as opposed to thermal) energy source terms for the neutrals, ions, and electrons. We first observe that the neutral fluid energy equation (11) of FPH85 is identical with our (2.16) provided one makes the identification

$$B_n = G_n + F_{nz}v_{nz} - \frac{1}{2}S_n v_{nz}^2. \quad (5.1)$$

This interpretation of  $B_n$  will be adopted, since otherwise equation (11) of FPH85 would be invalid.

For the case of ion–electron radiative recombination  $I^+ + e^- \rightarrow A + h\nu$  at a rate per volume  $N_{nl} = an_I n_e$ , FPH85 give (their equations 25 and 27)

$$B_{nl} = N_{nl} \{ \frac{1}{2}m_A v_i^2 + \frac{5}{4}k(T_i + T_e) \}.$$

According to our analysis above, however, we find that

$$G_{nl} + F_{nl,z}v_{nz} - \frac{1}{2}S_{nl} v_{nz}^2 = N_{nl} ( \frac{1}{2}m_A v_i^2 + \frac{3}{2}kT_i ). \quad (5.2)$$

For dissociative recombination, FPH85 (equations 25, 27, and 31) give

$$B_n = N_{nl} \{ \frac{1}{2}m_I v_i^2 + \frac{5}{4}k(T_i + T_e) + \Delta E \},$$

whereas we find

$$G_{n,\lambda} + F_{n,\lambda} v_{nz} - \frac{1}{2}S_{n,\lambda} v_{nz}^2 = N_{n,\lambda} ( \frac{1}{2}m_I v_i^2 + \frac{3}{2}kT_i + kT_e + \Delta E ). \quad (5.3)$$

It is clear that our results for the heating effect of ion–electron recombination differ significantly from the formulae given by FPH85.

## 5.3 VALIDITY OF THE APPROXIMATIONS

### 5.3.1 Maxwellian velocity distributions

The derivation of the MHD equations given in Section 2 assumes that the stress tensor (Landau & Lifshitz 1959) is isotropic: i.e., diagonal, with equal velocity dispersions in the  $x$ ,  $y$ , and  $z$  directions. To what extent is this assumption valid? Evaluation of various source terms in Sections 3 and 4 further relied on the assumption that the velocity distribution functions could be approximated by Maxwellian distributions. How good is this approximation?

Let  $\tau_{\text{flow}} \approx L/v_s$  be the time-scale for the fluid to flow a length  $L$  over which physical conditions

\* This error in the MHD equations of FPH85 appears to have only very minor numerical consequences in MHD shocks in molecular clouds of low fractional ionization, such as those studied by FPH85. This is because adiabatic compression contributes only a small fraction of the heating of the electrons and ions – in the centre of the shock transition region, heating of the ions is dominated by collisions with streaming neutrals, and heating of the electrons is primarily due to Coulomb scattering by the hot ions.

change appreciably. For steady, plane-parallel  $C$ -type MHD shocks,  $L$  is of order (D80).

$$L \approx \frac{(m_n + m_i) B_0^2}{\pi \rho_{i0} \rho_{n0} \langle \tilde{\sigma}_{in} v \rangle v_s} \quad (5.4)$$

where  $B_0$  is the preshock transverse magnetic field,  $\rho_{i0}$  and  $\rho_{n0}$  are the preshock densities of ions and neutrals, and  $\langle \tilde{\sigma}_{in} v \rangle$  is the ion–neutral momentum transfer rate coefficient.

Let  $\tau_{f\beta}$  be the mean time, for a typical particle of fluid  $f$ , between collisions with a particle of species  $\beta$ . Then

$$\tau_{ff} = \left( \sum_{\beta \in f} \tau_{f\beta}^{-1} \right)^{-1} \quad (5.5)$$

is the relaxation time for fluid  $f$ . Since elastic scattering of  $f$  by  $f$  will tend to bring about a Maxwellian distribution for  $f$ , it is clear that

$$\frac{\tau_{ff}}{\tau_{flow}} \ll 1, \quad f \in \{n, i, e\} \quad (5.6)$$

is a *necessary* condition for fluid  $f$  to have a near-Maxwellian velocity distribution. If fluid  $g$  is streaming through fluid  $f$  with a velocity  $(\vec{v}_g - \vec{v}_f)$  which is appreciable compared to the velocity dispersion of fluid  $f$ , then a second necessary condition is that the rate of heating per volume be small compared to the thermal energy density divided by the self-relaxation time  $\tau_{ff}$ :

$$\sum_{\beta \in g} \frac{m_f m_\beta^2 |\vec{v}_\beta - \vec{v}_f|^2}{(m_f + m_\beta)^2 k T_f} \frac{\tau_{ff}}{\tau_{f\beta}} \ll 1. \quad (5.7)$$

Note that (5.7) is not a *sufficient* condition: one could have infrequent but violent collisions (e.g.,  $\tau_{ff}/\tau_{f\beta} = 10^{-2}$ ,  $m_f m_\beta^2 |\vec{v}_\beta - \vec{v}_f|^2 / (m_f + m_\beta)^2 = 10 k T_f$ ) which would result in a pronounced non-Maxwellian tail to the velocity distribution.

For the neutrals, using (5.4) with  $\langle \tilde{\sigma}_{in} v \rangle \approx 2 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$  we obtain

$$\frac{\tau_{nn}}{\tau_{flow}} \approx 2 \left( 1 + \frac{m_n}{m_i} \right)^{-1} \left( \frac{4\pi \rho_{n0} v_s^2}{B_0^2} \right) \left( \frac{T_n}{10^3 \text{ K}} \right)^{-1/2} \frac{n_i}{n_n}, \quad (5.8)$$

and

$$\frac{\tau_{nn}}{\tau_{ni}} \approx 3 \left( \frac{T_n}{10^3 \text{ K}} \right)^{-1/2} \frac{n_i}{n_n}, \quad (5.8)$$

where we have assumed a neutral–neutral scattering cross-section  $\sim 10^{-15} \text{ cm}^2$ . Streaming electrons will have little effect on the neutrals because  $m_e \ll m_n$ . Thus in flows with  $(4\pi \rho_{n0} v_s^2 / B_0^2) \leq 10^3$  and low fractional ionization  $n_i / n_n \leq 10^{-3.5}$  the conditions (5.6) and (5.7) are both satisfied: neither compression of the neutrals nor collisions with streaming ions will significantly distort the velocity distribution function of the neutrals.

For the electrons we find

$$\frac{\tau_{ee}}{\tau_{flow}} \approx 3 \times 10^{-7} \left( \frac{T_e}{10^3 \text{ K}} \right)^{1/2} \left[ \frac{4\pi \rho_{n0} v_s^2}{B_0^2} \right], \quad (5.10)$$

where we have assumed  $\ln \Lambda \approx 25$  in evaluating the electron–electron collision time (Spitzer 1962). Since the factor in square brackets probably does not exceed  $10^3$ , the velocity distribution function for the electrons will be close to Maxwellian.

Evaluating the condition (5.7) for the ions we find

$$\frac{m_i m_n^2 |\vec{v}_i - \vec{v}_n|^2}{(m_i + m_n)^2 k T_i} \frac{\tau_{ii}}{\tau_{in}} \approx 6 \times 10^{-4} \frac{n_n}{n_i} \left( \frac{|\vec{v}_i - \vec{v}_n|}{5 \text{ km s}^{-1}} \right)^2 \left( \frac{T_i}{10^4 \text{ K}} \right)^{1/2}, \quad (5.11)$$

where we have assumed  $\ln \Lambda = 25$ ,  $m_i = 12 m_H$ , and  $m_n = 1.5 m_H$ . It will turn out that in many flows, (5.11) is *not* small compared to unity, so that condition (5.7) for the ions is not satisfied. For example, in the central regions of the  $v_s = 25 \text{ km s}^{-1}$  shock waves shown in Figs 1, 2, and 3 of DRD83 the fractional ionization  $n_i/n_n < 2 \times 10^{-4}$ ,  $|\vec{v}_n - \vec{v}_i| > 15 \text{ km s}^{-1}$ , and  $T_i > 10^4 \text{ K}$ , so that the right-hand side of equation (5.11) exceeds  $\sim 30$ . Thus we see that strongly non-Maxwellian ion velocity distributions may be present in interstellar C-type MHD shock waves. For any plausible magnetic field strength the gyroperiod will always be short enough to maintain azimuthal symmetry of the ion velocity distribution with respect to the local field direction, but the velocity distribution in the two directions perpendicular to  $\vec{B}$  may differ greatly from the distribution parallel to  $\vec{B}$ . The energy distribution may also be strongly non-Maxwellian. Such departures from a thermal velocity distribution may have important implications for endothermic ion-molecule reactions (e.g.,  $\text{C}^+ + \text{H}_2 + 0.4 \text{ eV} \rightarrow \text{CH}^+ + \text{H}$ ), a question which merits further investigation.

### 5.3.2 Viscous stresses

The derivation of the MHD equations given in Section 2 assumes that viscous stresses are negligible. We have seen above that the neutrals and electrons in C-type shocks will have velocity distributions which are close to a Maxwellian distribution (for which the viscous stresses vanish). For the ions, on the other hand, we have seen that the velocity distribution function may in some cases be highly anisotropic. Our estimates for the ‘pressure’ forces due to the ions are therefore somewhat inaccurate; the ion viscous stresses may sometimes be comparable to the ‘pressure’ stress. Nevertheless, the MHD equations derived neglecting viscous stresses remain a good approximation, because a low fractional ionization ensures that the ion pressure is not dynamically important.

We conclude that the neglect of viscous stresses and the use of equations (2.9, 2.10, 2.15) are satisfactory approximations *outside of ‘jump’ fronts* for MHD shocks in low-fractional ionization interstellar clouds. Within a jump front, if present, the viscous stresses are large, but the detailed structure of the viscous shock transition is not generally of interest, and it can normally be treated as a discontinuity, the usual ‘jump conditions’ being used to connect the fluid variables across the jump front.

### 5.3.3 Finite electrical conductivity

It has been assumed in Section 2 that the conductivity of the plasma is essentially infinite, resulting in ‘freezing’ of the flux lines into the plasma. For finite conductivity, the electric current is  $\vec{J} = \sigma_{\text{cond}}(\vec{E} - \vec{v}_i \times \vec{B}/c)$ . Assuming  $\partial/\partial t = 0$ , and using Maxwell’s equations, one obtains

$$\nabla \times (\vec{B} \times \vec{v}_i) = \frac{c^2}{4\pi} \nabla \times \left( \frac{\nabla \times \vec{B}}{\sigma_{\text{cond}}} \right), \quad (5.12)$$

so that the fractional error in the flux-freezing equation (2.12) is negligible provided  $\sigma_{\text{cond}} \gg c^2/4\pi v_s L$ , where  $L$  is the characteristic length scale for variation in  $\vec{B}$ . Using equation (5.4) to estimate  $L$ , and assuming  $B_0 \approx 10^{-6} (n_{n0}/\text{cm}^{-3})^{1/2} \text{ gauss}$  and  $\langle \tilde{\sigma}_{\text{in}} v \rangle \approx 2 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ , this



implies that the conductivity must satisfy the condition

$$\sigma_{\text{cond}} \geq 9 \times 10^{-3} \left( \frac{n_{i0}}{0.01 \text{ cm}^{-3}} \right) \text{ s}^{-1}. \quad (5.13)$$

The electron contribution to the conductivity, considering scattering by both ions and neutrals, is approximately

$$\begin{aligned} \sigma_{\text{cond}} &= \frac{0.59 (kT_e)^{3/2}}{e^2 m_e^{1/2} \ln \Lambda} \left\{ 1 + 1.9 \frac{n_n \tilde{\sigma}_{\text{en}} (kT_e)^2}{n_e e^4 \ln \Lambda} \right\}^{-1} \\ &= 5.5 \times 10^{12} \left( \frac{T_e}{10^4 \text{ K}} \right)^{3/2} \left\{ 1 + 2.7 \times 10^{-3} \frac{n_n}{n_e} \left( \frac{T_e}{10^4 \text{ K}} \right)^2 \right\}^{-1} \text{ s}^{-1}, \end{aligned} \quad (5.14)$$

where we have assumed  $\ln \Lambda \approx 25$  and an electron–neutral scattering cross-section  $\tilde{\sigma}_{\text{en}} \approx 10^{-15} \text{ cm}^2$ . It therefore is clear that the perfect conductivity approximation is valid even for very low fractional ionization.

It has also been assumed in the derivation of the equations that the electrons and ions share the same bulk flow velocity. Since currents must be present to sustain the magnetic field gradients, it is clear that there must be differences in the mean velocities of the ions and electrons. However, using equation (5.4) to estimate the length scale for magnetic field compression, we find that the velocity difference between ions and electrons is only

$$|\vec{v}_i - \vec{v}_e| \approx 0.06 \left( \frac{n_{n0}}{\text{cm}^{-3}} \right)^{1/2} \left( \frac{v_s}{10 \text{ km s}^{-1}} \right) \text{ cm s}^{-1}, \quad (5.15)$$

which is clearly negligible from the standpoint of energy or momentum conservation.

## 6 Conclusions

The principal results of this paper are:

(i) A rigorous derivation has been given for the conservation laws for mass, number, momentum, and energy in a multicomponent, reacting fluid flow, including neutrals, ions, electrons, and magnetic field. No restriction has been made concerning the orientation of the magnetic field relative to the direction of propagation of the shock. The results of D80 and DRD83 are recovered for the special case of magnetic field transverse to the direction of shock propagation. The electron energy equation used by FPH85 is shown to be incorrect.

(ii) General expressions are presented for the momentum and energy ‘source terms’ associated with both non-reactive and reactive scattering.

(iii) For the case of elastic scattering, we give exact results, as well as simple approximations, for the energy and momentum source terms for two special cases of the momentum transfer cross-section:  $\tilde{\sigma} \propto v^{-1}$  and  $\tilde{\sigma} = \text{constant}$ .

(iv) The source terms associated with several specific ‘chemical’ processes, such as photoionization, recombination, and ion–molecule exchange reactions, are determined. Comparison is made with the results of FPH85.

(v) The validity of the MHD formulation given here – in particular, the neglect of viscous stresses, and the assumption of perfect conductivity – are examined. These approximations are shown to be highly valid for shock waves in interstellar clouds.

(vi) It is shown that ion–neutral collisions can in some cases result in non-Maxwellian velocity distributions for the ions. This may have implications for endothermic ion–molecule reactions.



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## Appendix A: Momentum source term $\vec{F}_{\alpha\lambda}$

Let  $\lambda$  denote elastic scattering of species  $\alpha$  and  $\beta$ . Let  $\vec{w}_{\alpha i}$  and  $\vec{w}_{\beta i}$  denote the velocities of particles  $\alpha$  and  $\beta$  prior to scattering, and let  $\vec{w}_{\alpha f}$  and  $\vec{w}_{\beta f}$  be the corresponding velocities after scattering. Let  $d\sigma/d\Omega$  be the differential scattering cross-section in the centre-of-mass frame. For elastic scattering, the outgoing velocities  $\vec{w}_{\alpha f}$  and  $\vec{w}_{\beta f}$  are fully determined by the initial velocities and the scattering angle. Then the rate per volume of momentum transfer to species  $\alpha$  is

$$\vec{F}_{\alpha\lambda} \equiv n_{\alpha} n_{\beta} \int d\vec{w}_{\alpha i} \varphi_{\alpha}(\vec{w}_{\alpha i}) \int d\vec{w}_{\beta i} \varphi_{\beta}(\vec{w}_{\beta i}) |\vec{w}_{\alpha i} - \vec{w}_{\beta i}| \int d\Omega \frac{d\sigma}{d\Omega} m_{\alpha} (\vec{w}_{\alpha f} - \vec{w}_{\alpha i}),$$

where  $\varphi_{\alpha}$  and  $\varphi_{\beta}$  are the velocity distribution functions for species  $\alpha$  and  $\beta$ . The momentum transfer cross-section  $\tilde{\sigma}(w_{\text{rel}})$  for relative velocity  $w_{\text{rel}}$  is defined by

$$\int d\Omega \frac{d\sigma}{d\Omega} m_{\alpha} (\vec{w}_{\alpha f} - \vec{w}_{\alpha i}) = \tilde{\sigma}(w_{\text{rel}}) \frac{m_{\alpha} m_{\beta}}{m_{\alpha} + m_{\beta}} (\vec{w}_{\beta i} - \vec{w}_{\alpha i}).$$

If we assume Maxwellian velocity distributions of the form

$$\varphi_{\alpha}(\vec{w}_{\alpha}) = \left( \frac{m_{\alpha}}{2\pi k T_{\alpha}} \right)^{3/2} \exp \left( - \frac{m_{\alpha} |\vec{w}_{\alpha} - \vec{v}_{\alpha}|^2}{2k T_{\alpha}} \right),$$

where  $\vec{v}_{\alpha}$  is the mean flow velocity, then straightforward though tedious integration yields the result (3.1) for the momentum transfer rate  $\vec{F}_{\alpha\lambda}$ .

## Appendix B: Heat source term $G_{\alpha\lambda}$

Using the same notation as Appendix A, the rate of increase of thermal energy per volume of species  $\alpha$  as the result of a scattering process  $\lambda$  is

$$G_{\alpha\lambda} \equiv n_{\alpha} n_{\beta} \int d\vec{w}_{\alpha i} \varphi_{\alpha}(\vec{w}_{\alpha i}) \int d\vec{w}_{\beta i} \varphi_{\beta}(\vec{w}_{\beta i}) |\vec{w}_{\alpha i} - \vec{w}_{\beta i}| \int d\Omega \frac{d\sigma}{d\Omega} \left\{ \frac{1}{2} m_{\alpha} (w_{\alpha f}^2 - w_{\alpha i}^2) \right\} - \vec{f}_{\alpha\lambda} \cdot \vec{v}_{\alpha}.$$

For elastic scattering, Maxwellian velocity distribution functions  $\varphi_{\alpha}$  and  $\varphi_{\beta}$ , and the momentum transfer cross-section  $\tilde{\sigma}$  of Appendix A, routine though tedious integration yields the general result (3.7).