Multicomponent diffusion in two-temperature magnetohydrodynamics

J. D. Ramshaw and C. H. Chang

Idaho National Engineering Laboratory, P. O. Box 1625, Idaho Falls, Idaho 83415

(Received 22 November 1995)

A recent hydrodynamic theory of multicomponent diffusion in multitemperature gas mixtures [J. D. Ramshaw, J. Non-Equilib. Thermodyn. **18**, 121 (1993)] is generalized to include the velocity-dependent Lorentz force on charged species in a magnetic field **B**. This generalization is used to extend a previous treatment of ambipolar diffusion in two-temperature multicomponent plasmas [J. D. Ramshaw and C. H. Chang, Plasma Chem. Plasma Process. **13**, 489 (1993) to situations in which **B** and the electrical current density are nonzero. General expressions are thereby derived for the species diffusion fluxes, including thermal diffusion, in both single- and two-temperature multicomponent magnetohydrodynamics (MHD). It is shown that the usual zerofield form of the Stefan-Maxwell equations can be preserved in the presence of **B** by introducing generalized binary diffusion tensors dependent on **B**. A self-consistent effective binary diffusion approximation is presented that provides explicit approximate expressions for the diffusion fluxes. Simplifications due to the small electron mass are exploited to obtain an ideal MHD description in which the electron diffusion coefficients drop out, resistive effects vanish, and the electric field reduces to a particularly simple form. This description should be well suited for numerical calculations. $[$1063-651X(96)06406-9]$

PACS number(s): 52.25.Dg, 52.25.Fi, 52.25.Vy, 52.25.Ya

I. INTRODUCTION

Theoretical work in plasma physics is frequently restricted to two- or three-component plasmas for simplicity. Real plasmas, however, are generally multicomponent mixtures in which several different types of ions and neutral atoms are present in different and varying concentrations. Such plasmas are largely intractable analytically, but there is a growing interest in studying them by means of detailed numerical simulations $[1-3]$. Such simulations must necessarily be based on general theoretical relations valid for an arbitrary mixture of *N* components. Moreover, these relations must be expressed in a form suitable for numerical implementation and solution.

Single-fluid or magnetohydrodynamic (MHD) descriptions are commonly used to represent low-frequency dynamical phenomena in plasmas $[4-6]$. However, the term ''single fluid'' is somewhat misleading, since the plasma must still be treated as a mixture of different components or species, the concentrations of which appear as separate dependent variables in the description. Each such component satisfies a continuity equation of the form

$$
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}) = -\nabla \cdot \mathbf{J}_i + \dot{\rho}_i^c,
$$
 (1)

where ρ_i is the partial mass density (mass per unit volume) of species i , \mathbf{J}_i is the diffusive mass flux of species i relative to the mass-weighted velocity **u** of the plasma as a whole, and $\dot{\rho}_i^c$ represents the rate of change of ρ_i due to chemical reactions, including ionization and recombination processes. The plasma is a ''single fluid'' only in the sense that **u** is determined by a single momentum equation, but constitutive relations for the diffusion fluxes J_i are still required to determine the species densities ρ_i and close the system. Only in very special situations can the ρ_i be determined by means of other relations, without knowledge of the **J***ⁱ* . Situations of this type include the common textbook cases of fully ionized two-component plasmas and three-component plasmas in ionization equilibrium, but in a generic sense such cases are highly exceptional.

Multicomponent diffusion is therefore an essential but somewhat neglected ingredient in MHD descriptions of partially or fully ionized plasmas. Unfortunately, the standard kinetic theory of gases $[7-9]$ requires nontrivial generalizations in order to describe the diffusion of charged species in a magnetic field, especially in two-temperature plasmas exhibiting persistent temperature differences between the electrons and heavy particles. These generalizations have been pursued by several intrepid authors $[9-16]$. However, such treatments quite understandably tend to be highly formal, and the results are not in general well suited to the actual numerical evaluation of the diffusion fluxes.

It has been shown recently that the complications arising from two (or multiple) temperatures are much more easily handled within the framework of a hydrodynamic theory of diffusion $\left[17-19\right]$. This theory was subsequently used to develop a tractable formulation for ambipolar diffusion in twotemperature plasmas in zero magnetic field $[20]$. The hydrodynamic approach is equally amenable to the inclusion of magnetic field effects, and the main purpose of the present paper is to extend the formulation of $[20]$ to cases in which the magnetic field **B** and electrical current density J_q are nonzero. However, this extension requires a reconsideration of the hydrodynamic theory of Ref. $[17]$, which was originally developed under the tacit assumption that velocitydependent forces are absent. This restriction must be removed so that the velocity-dependent Lorentz force may be included in the formulation. Fortunately, the required modifications are straightforward, and we thereby obtain generalized Stefan-Maxwell (SM) equations, which are twotemperature generalizations of those previously given for single-temperature plasmas in a magnetic field with thermal diffusion neglected $[8,10]$. These equations constitute a com-

1063-651X/96/53(6)/6382(7)/\$10.00 53 6382 © 1996 The American Physical Society

plete tractable description of multicomponent diffusion in two-temperature plasmas in a magnetic field. This description should be well suited for practical applications.

The generalized SM equations contain two types of phenomenological coefficients, namely, frictional and thermophoretic force coefficients. Determination of the actual numerical values of these coefficients falls outside the scope of the present theory. This problem has unfortunately not been solved in full generality, but reasonable values for these coefficients can generally be inferred from the results of simple $[17–19,21]$ or more sophisticated $[8–15,22]$ kinetic theories. Alternatively, these coefficients may be regarded as empirical parameters to be obtained from experiments.

The paper is organized as follows. In Sec. II we revisit the hydrodynamic theory in order to incorporate the modifications needed to treat velocity-dependent forces. These modifications result in generalized SM equations for either singleor two-temperature plasmas in a magnetic field. These are the fundamental equations on which the remainder of the development is based. They have a somewhat more general structure than the SM equations for $B=0$, which manifestly depend only on differences between velocities of different species. In Sec. III, however, we show that the generalized SM equations may nevertheless be cast into the same form as those for $B=0$ by introducing generalized binary diffusion tensors dependent on **B**. In Sec. IV we present a selfconsistent effective binary diffusion (SCEBD) approximation $[23,24]$, which leads to explicit approximate expressions for the diffusion fluxes. In Sec. V we explore the simplifications that result in the ideal MHD limit of zero electron mass. In this limit the electron diffusion coefficients drop out, resistive effects vanish, and the electric field reduces to a particularly simple form. This description should be well suited for numerical calculations, as the very large electron diffusivities no longer appear and therefore cannot give rise to stiffness or ill conditioning. Section VI contains a few concluding remarks.

II. TWO-TEMPERATUE STEFAN-MAXWELL EQUATIONS IN A MAGNETIC FIELD

Just as in $[17]$, we begin by writing the momentum equations for the individual species *i*, which take the familiar form

$$
\rho_i \frac{D_i \mathbf{u}_i}{Dt} = -\nabla p_i + \rho_i \mathbf{F}_i + \sum_j \mathbf{F}_{ij},
$$
\n(2)

where \mathbf{u}_i is the mean velocity of species *i*, $D_i/Dt = \partial/\partial t + \mathbf{u}_i \cdot \nabla$, p_i is the partial pressure of species *i*, \mathbf{F}_i is the body force per unit mass acting on species *i*, \mathbf{F}_{ii} = $-\mathbf{F}_{ji}$ is the mean force per unit volume of species *j* on species *i*, the *j* summation extends over the *N* components in the mixture, and viscous effects have been neglected. Attention is restricted to ideal gases, for which

$$
p_i = \rho_i k_B T_i / m_i, \qquad (3)
$$

where k_B is Boltzmann's constant, and T_i and m_i are, respectively, the temperature and particle mass of species *i*. In the present context, the temperatures of all the heavy species are presumed equal, but possibly different from the temperature of the free electrons. Thus $T_i = T$ for $i \neq e$ and $T_i = T_e$ for $i = e$, where the subscript *e* symbolically denotes the species index of the free electrons. The mass-weighted velocity **u** of the mixture is related to the individual species velocities by ρ **u**= $\Sigma_i \rho_i$ **u**_{*i*}, where $\rho = \Sigma_i \rho_i$ is the total mass density of the plasma mixture. The species diffusion fluxes are then given by $\mathbf{J}_i = \rho_i(\mathbf{u}_i - \mathbf{u})$.

The body forces \mathbf{F}_i are taken to be of the form

$$
\mathbf{F}_i = \mathbf{g} + q_i \left(\mathbf{E} + \frac{1}{c} \mathbf{u}_i \times \mathbf{B} \right),\tag{4}
$$

where **g** is the acceleration of gravity, q_i is the charge per unit mass of species i , \bf{E} is the electric field, and c is the speed of light. We shall presume that \mathbf{F}_{ij} is of the general form $[17]$

$$
\mathbf{F}_{ij} = \boldsymbol{\alpha}_{ij} \cdot (\mathbf{u}_j - \mathbf{u}_i) + \boldsymbol{\beta}_{ij} \cdot \nabla \ln T_j - \boldsymbol{\beta}_{ji} \cdot \nabla \ln T_i, \qquad (5)
$$

where α_{ij} and β_{ij} are frictional and thermophoretic force coefficients, respectively, which now become tensors due to the presence of \bf{B} [10]. The former coefficients are symmetric in (i, j) , whereas the latter are not [17]. Approximate expressions for these coefficients when $B=0$ are given in Refs. $[17–19]$. Corresponding expressions for nonzero **B** have apparently not been derived in full generality, but results are available in particular cases $[10,13,21]$.

Multifluid dynamical descriptions of the present type typically reduce to a diffusional description when the friction coefficients are large $[17,25]$. This is the situation of present interest. The effect of large friction is to prevent and/or destroy any large differences between species velocities, so that all of the individual species velocities **u***ⁱ* become very nearly equal to the mass-averaged velocity **u**. It then becomes a good approximation to replace $D_i \mathbf{u}_i / Dt$ by $D\mathbf{u}/Dt$ in Eq. (2), where $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the standard convective derivative. Equation (2) then becomes

$$
\rho_i \frac{D \mathbf{u}}{Dt} = -\nabla p_i + \rho_i \mathbf{F}_i + \sum_j \mathbf{F}_{ij} \,. \tag{6}
$$

One might at first think that consistency would require the simultaneous replacement of \mathbf{u}_i by \mathbf{u} in Eq. (4). However, this would further reduce the accuracy of the approximation, since for large but finite values of the α_{ij} , the derivatives of the \mathbf{u}_i may be expected to be more nearly equal than the \mathbf{u}_i themselves. (That is to say, the relative or percentage deviations of the $D_i \mathbf{u}_i / Dt$ from $D \mathbf{u}/Dt$ will generally be smaller than the corresponding deviations of the \mathbf{u}_i from \mathbf{u}_i , so that less error is introduced by neglecting the former deviations than the latter. Note in particular that if the \mathbf{u}_i differ by small constant amounts, the differences between their derivatives are zero.) We therefore retain Eq. (4) in its present form, in accordance with the usual practice $[8,10]$. We also remark that the approximation leading to Eq. (6) does *not* imply a corresponding restriction to small differences between the electron and heavy-particle temperatures, since the characteristic or relaxation time scale for temperature equilibration is much slower than that for velocity equilibration $[6,10]$.

The total momentum equation for the plasma is obtained by summing Eq. (6) over all species, with the result

$$
\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \sum_{i} \rho_i \mathbf{F}_i = -\nabla p + \rho \mathbf{g} + \frac{1}{c} \mathbf{J}_q \times \mathbf{B}, \qquad (7)
$$

where $J_q = \sum_i \rho_i q_i \mathbf{u}_i$ is the electrical current density, and use has been made of Eq. (4) and the neutrality condition $\sum_i \rho_i q_i = 0$, which is an identity in MHD [4,5]. Equation (7) is of course simply the standard MHD momentum equation $[4–6]$. This equation determines **u**, which should therefore be regarded as a given quantity rather than a derived quantity determined by the \mathbf{u}_i . That is to say, \mathbf{u} is a constraint on the \mathbf{u}_i rather than a consequence of the \mathbf{u}_i . Similarly, the current density J_a in MHD is determined by Ampere's law, and should also be regarded as a given quantity that represents a second constraint on the **u***ⁱ* .

Combining Eqs. $(5)-(7)$, we obtain

$$
\sum_{j} \boldsymbol{\alpha}_{ij} \cdot (\mathbf{u}_{j} - \mathbf{u}_{i}) + \frac{\rho_{i} q_{i}}{c} \mathbf{u}_{i} \times \mathbf{B} = \mathbf{G}_{i},
$$
 (8)

where

$$
\mathbf{G}_i = p \nabla z_i + (z_i - y_i) \nabla p + \frac{y_i}{c} \mathbf{J}_q \times \mathbf{B} - \rho_i q_i \mathbf{E} - \boldsymbol{\gamma}_i, \qquad (9)
$$

$$
\gamma_i = \sum_j \left(\boldsymbol{\beta}_{ij} \cdot \nabla \ln T_j - \boldsymbol{\beta}_{ji} \cdot \nabla \ln T_i \right), \tag{10}
$$

 $z_i = p_i / p$, and $y_i = \rho_i / \rho$. Equation (8) is a system of generalized SM equations for two-temperature plasmas in a magnetic field. Their resemblance to the standard SM equations $[17]$ can be increased by introducing binary diffusion tensors defined by

$$
\mathsf{D}_{ij} = p z_i z_j \boldsymbol{\alpha}_{ij}^{-1} \,. \tag{11}
$$

However, the friction coefficients α_{ij} are often more convenient to work with $[13]$, so we shall retain them in preference to the D_{ij} .

Equation (8) is reminiscent of a system of generalized SM-like equations derived from kinetic theory by Burgers [13]. The essential difference between the two formulations is that we have decomposed the forces \mathbf{F}_{ij} into frictional terms and terms proportional to temperature gradients, whereas Burgers effectively decomposes them into frictional terms and terms proportional to species heat fluxes. The latter obey a system of SM-like equations of their own, which are coupled to the SM equations for the diffusion velocities. This greatly increases the complexity of the description, which correspondingly increases the barrier to practical applications. Nevertheless, the two formulations are in principle equivalent if all terms are retained and consistently evaluated. The relation between them can be simply seen by observing that the present formulation could evidently have been reached by the alternate route of further decomposing Burgers' heat flux terms into parts proportional to species velocities and temperature gradients, and absorbing the former into the α_{ij} .

Only $N-1$ of the SM equations (8) are linearly independent (where *is the number of species in the plasma, in*cluding the free electrons), as their sum over species reduces to an identity. The constraints imposed by the given values of **u** and J_q provide two additional equations, so that there are $N+1$ equations in the $N+1$ unknowns \mathbf{u}_i and **E**. (The magnetic field **B** may also be regarded as known, since it is determined by Faraday's Law in MHD $[4-6]$.) The solution of these equations therefore determines **E** as well as the \mathbf{u}_i or J_i , and this implicitly determines the relation between E and J_q ; i.e., Ohm's law. It follows that Ohm's law is not an independent constitutive relation in multicomponent MHD, but is rather a consequence and combination of the constitutive relations for the species diffusion fluxes $[10,13]$. Thus it is not in general possible to express J_q directly in terms of **E**, or *vice versa*, without determining the J_i .

In contrast to the SM equations in zero magnetic field, Eq. ~8! no longer depends on velocity differences alone but now involves absolute velocities through the $\mathbf{u}_i \times \mathbf{B}$ term. The SM equations therefore have a somewhat different mathematical structure in the presence of **B**. However, their structure can nevertheless be restored to its $\mathbf{B} = 0$ form by suitable manipulations, as shown in the next section.

III. GENERALIZED BINARY DIFFUSION TENSORS

Using the neutrality condition, we readily find that the current density can be rewritten in the form

$$
\mathbf{J}_q = \sum_j \ \rho_j (q_i + q_j) (\mathbf{u}_j - \mathbf{u}_i) + \rho q_i (\mathbf{u}_i - \mathbf{u}), \tag{12}
$$

which combines with Eqs. (8) and (9) to yield

$$
\sum_{j} \left[\boldsymbol{\alpha}_{ij} + \frac{\rho_i \rho_j}{\rho c} (q_i + q_j) \mathbf{B} \right] \cdot (\mathbf{u}_j - \mathbf{u}_i) = \mathbf{G}_i^*, \qquad (13)
$$

where **B** is the antisymmetric tensor defined operationally by $\mathbf{B} \cdot \mathbf{v} = \mathbf{B} \times \mathbf{v}$ for any vector **v** (or equivalently by $\mathbf{B} = \mathbf{B} \times \mathbf{U}$, where U is the unit tensor), and the modified driving forces \mathbf{G}_i^* are defined by

$$
\mathbf{G}_{i}^{*} = \mathbf{G}_{i} - \frac{y_{i}}{c} (\mathbf{J}_{q} + \rho q_{i} \mathbf{u}) \times \mathbf{B}
$$

= $p \nabla z_{i} + (z_{i} - y_{i}) \nabla p - \rho_{i} q_{i} \left(\mathbf{E} + \frac{1}{c} \mathbf{u} \times \mathbf{B} \right) - \gamma_{i}.$ (14)

The quantity $\mathbf{E} + (1/c)\mathbf{u} \times \mathbf{B}$ is of course simply the electric field in a coordinate system moving with the fluid velocity **u**. All of the remaining dependence on **B** has been absorbed into the tensor coefficients in the left member of Eq. (13) . Comparison with Eq. (8) shows that these coefficients may be regarded as generalized friction coefficients defined by

$$
\boldsymbol{\alpha}_{ij}^* = \boldsymbol{\alpha}_{ij} + \frac{\rho_i \rho_j}{\rho c} (q_i + q_j) \mathbf{B},\tag{15}
$$

corresponding to which we may also define generalized binary diffusivity tensors by

$$
\mathbf{D}_{ij}^* = p z_i z_j (\boldsymbol{\alpha}_{ij}^*)^{-1} = p z_i z_j \bigg[\boldsymbol{\alpha}_{ij} + \frac{\rho_i \rho_j}{\rho c} (q_i + q_j) \mathbf{B} \bigg]^{-1}.
$$
\n(16)

By symmetry, the α_{ij} will be of the form [10]

$$
\boldsymbol{\alpha}_{ij} = \alpha_{ij}^{\parallel} \mathbf{b} \mathbf{b} + \alpha_{ij}^{\perp} (\mathbf{U} - \mathbf{b} \mathbf{b}), \qquad (17)
$$

where $\mathbf{b} = \mathbf{B}/|\mathbf{B}|$. The inverse tensor in Eq. (16) can then be evaluated in the usual way [6]. Notice that $\alpha_{ji}^* = \alpha_{ij}^*$ and D_{ii}^* = D_{ii}^* by construction.

Combining Eqs. (13) and (15) , we obtain the SM equations in the equivalent but simpler form

$$
\sum_{j} \; \mathbf{a}_{ij}^* \cdot (\mathbf{u}_j - \mathbf{u}_i) = \mathbf{G}_i^* \; . \tag{18}
$$

In this form, the SM equations once again involve only differences between species velocities, just as they do for $B=0$.

IV. THE SELF-CONSISTENT EFFECTIVE BINARY DIFFUSION APPROXIMATION

The SM equations (8) or (18) constitute a linear system of equations for the species velocities. SCEBD approximations are often used to avoid solving such systems $[17,20,23,24]$. The SCEBD approximation has recently been reconsidered and reformulated as a systematic constructive approximation to the SM equations $[24]$. This reformulation removes an ambiguity in earlier versions of the approximation, as well as significantly increasing the accuracy. We now proceed to generalize this improved SCEBD approximation to the present context.

The development of Ref. $[24]$ is based on a systematic approximation to the friction coefficients α_{ij} , so the appropriate starting point for present purposes is Eq. (8) , which may be rewritten in the form

$$
\left(\boldsymbol{\alpha}_i + \frac{\rho_i q_i}{c} \mathbf{B}\right) \cdot \mathbf{u}_i = -\mathbf{G}_i + \boldsymbol{\alpha}_i \cdot \mathbf{a}_i, \qquad (19)
$$

where

$$
\boldsymbol{\alpha}_i = \sum_j \; \boldsymbol{\alpha}_{ij} = \alpha_i^{\parallel} \mathbf{b} \mathbf{b} + \alpha_i^{\perp} (\mathbf{U} - \mathbf{b} \mathbf{b}), \tag{20}
$$

$$
\mathbf{a}_i = \boldsymbol{\alpha}_i^{-1} \cdot \sum_j \; \boldsymbol{\alpha}_{ij} \cdot \mathbf{u}_j \,, \tag{21}
$$

 $\alpha_i^{\parallel} = \sum_j \alpha_{ij}^{\perp}$, $\alpha_i^{\perp} = \sum_j \alpha_{ij}^{\perp}$, and we have adopted the definition $\alpha_{ii} \equiv 0$ for all *i* in order to avoid the restriction $j \neq i$ on the summations.

The essence of the SCEBD approximation is to approximate the α_{ij} in Eq. (21) in a form that permits an explicit approximate solution for the diffusion velocities \mathbf{u}_i [24]. The approximation previously used is given in Eq. (8) of Ref. $[24]$, of which the appropriate tensorial generalization is evidently

$$
\alpha_{ij} \cong w_i \cdot w_j (1 - \delta_{ij}). \tag{22}
$$

The factors W_i are now tensors, which we shall determine by requiring the approximation of Eq. (22) to be consistent with the correct values of the α_i [24]. Thus we combine Eqs. (20) and (22) to obtain

$$
\alpha_i = w_i \cdot (w - w_i), \qquad (23)
$$

where $w \equiv \sum_i w_i$.

The tensors W_i are implicitly defined by Eq. (23) . They will clearly be of the same tensorial form as the α_{ij} ; i.e.,

$$
\mathbf{w}_i = w_i^{\parallel} \mathbf{b} \mathbf{b} + w_i^{\perp} (\mathbf{U} - \mathbf{b} \mathbf{b}). \tag{24}
$$

It follows that $w_i \cdot w_j = w_j \cdot w_i$, which in turn implies that the approximation of Eq. (22) properly satisfies the condition $\alpha_{ij} = \alpha_{ji}$. (This is actually a special case of the general property that all tensors of the form T_{\parallel} **bb**+ T_{\perp} (U $-\mathbf{b}\mathbf{b}$)+ $T_\wedge(\mathbf{b}\times\mathbf{U})$ commute with each other. In what follows, this property will be freely used as needed without further comment.) According to Eqs. (17) , (20) , and (24) , Eqs. (22) and (23) may be decomposed into

$$
\alpha_{ij}^{\parallel} \cong w_i^{\parallel} w_j^{\parallel} (1 - \delta_{ij}), \tag{25}
$$

$$
\alpha_{ij}^{\perp} \cong w_i^{\perp} w_j^{\perp} (1 - \delta_{ij}), \tag{26}
$$

$$
\alpha_i^{\parallel} = w_i^{\parallel}(w^{\parallel} - w_i^{\parallel}), \tag{27}
$$

$$
\alpha_i^{\perp} = w_i^{\perp} (w^{\perp} - w_i^{\perp}), \qquad (28)
$$

where $w^{\parallel} = \sum_i w_i^{\parallel}$ and $w^{\perp} = \sum_i w_i^{\perp}$. Equations (27) and (28) unfortunately cannot be solved in closed form for the w_i^{\parallel} and w_i^{\perp} [24], so we shall subsequently propose suitable approximations for these quantities (or more precisely for the ratios $w_i^{\parallel}/w^{\parallel}$ and w_i^{\perp}/w^{\perp} , which are easier to approximate).

Combining Eqs. (21) and (22) , we obtain

$$
\boldsymbol{\alpha}_i \cdot \mathbf{a}_i = \mathbf{W}_i \cdot (\mathbf{W} \cdot \mathbf{a} - \mathbf{W}_i \cdot \mathbf{u}_i), \tag{29}
$$

where $w \cdot a \equiv \sum_j w_j \cdot u_j$. Equation (29) combines with Eqs. (19) and (23) to yield

$$
\left(\mathbf{w}_{i}\cdot\mathbf{w}+\frac{\rho_{i}q_{i}}{c}\mathbf{B}\right)\cdot\mathbf{u}_{i}=-\mathbf{G}_{i}+\mathbf{w}_{i}\cdot\mathbf{w}\cdot\mathbf{a}.
$$
 (30)

But according to Eq. (23) , we also have

$$
\mathbf{w}_i \cdot \mathbf{w} = \boldsymbol{\alpha}_i \cdot \boldsymbol{\Omega}_i^{-1} \,, \tag{31}
$$

where

$$
\Omega_i = U - W^{-1} \cdot W_i = \Omega_i^{\parallel} \mathbf{b} \mathbf{b} + \Omega_i^{\perp} (U - \mathbf{b} \mathbf{b}), \tag{32}
$$

with $\Omega_i^{\parallel} = 1 - w_i^{\parallel}/w^{\parallel}$ and $\Omega_i^{\perp} = 1 - w_i^{\perp}/w^{\perp}$. Equation (30) may therefore be rewritten in the form

$$
\mathbf{A}_i \cdot \mathbf{u}_i = -\mathbf{\Omega}_i \cdot \mathbf{G}_i + \mathbf{\alpha}_i \cdot \mathbf{a},\tag{33}
$$

where

$$
\mathsf{A}_{i} = \alpha_{i} + \frac{\rho_{i}q_{i}}{c}\mathsf{\Omega}_{i} \cdot \mathsf{B} = \alpha_{i} + \frac{\rho_{i}q_{i}\Omega_{i}^{\perp}}{c}\mathsf{B}.
$$
 (34)

Equation (33) may now be formally solved for \mathbf{u}_i , with the result

$$
\mathbf{u}_{i} = -\frac{1}{p_{i}} \mathbf{D}_{i} \cdot \mathbf{G}_{i} + \mathbf{M}_{i} \cdot \mathbf{a}, \qquad (35)
$$

where $M_i \equiv A_i^{-1} \cdot \alpha_i$, and the generalized effective binary diffusivities D*ⁱ* are defined by

$$
\mathsf{D}_{i} = p_{i} \mathsf{\Omega}_{i} \cdot \mathsf{A}_{i}^{-1} \,. \tag{36}
$$

Equation (35) expresses the **u**_{*i*} in terms of **a**, but **a** itself cannot be determined from the same equation, as only $N-1$ of these expressions are linearly independent. This may be seen by observing that the equivalent Eq. (30) reduces to an identity when summed over i . However, **a** may be determined and eliminated simply by requiring the \mathbf{u}_i to be consistent with the mass-weighted velocity $\mathbf{u} = \sum_i y_i \mathbf{u}_i$ $[23,24]$; i.e.,

$$
\mathbf{u} = -\sum_{i} \frac{y_i}{p_i} \mathbf{D}_i \cdot \mathbf{G}_i + \mathbf{M}_0 \cdot \mathbf{a}, \qquad (37)
$$

where $M_0 \equiv \sum_i y_i M_i$. We thereby obtain

$$
\mathbf{a} = \mathbf{M}_0^{-1} \cdot \left(\mathbf{u} + \sum_i \frac{y_i}{p_i} \mathbf{D}_i \cdot \mathbf{G}_i \right),\tag{38}
$$

which combines with Eq. (35) to yield

$$
\mathbf{u}_i = -\frac{1}{p_i} \mathbf{D}_i \cdot \mathbf{G}_i + \mathbf{M}_i \cdot \mathbf{M}_0^{-1} \cdot \left(\mathbf{u} + \sum_j \frac{y_j}{p_j} \mathbf{D}_j \cdot \mathbf{G}_j \right). \tag{39}
$$

The corresponding species diffusion fluxes are then given by

$$
\mathbf{J}_{i} = -\frac{\rho_{i}}{p_{i}} \mathbf{D}_{i} \cdot \mathbf{G}_{i} + \rho_{i} (\mathbf{M}_{i} \cdot \mathbf{M}_{0}^{-1} - \mathbf{U}) \cdot \mathbf{u}
$$

$$
+ y_{i} \mathbf{M}_{i} \cdot \mathbf{M}_{0}^{-1} \cdot \sum_{j} \frac{\rho_{j}}{p_{j}} \mathbf{D}_{j} \cdot \mathbf{G}_{j}, \qquad (40)
$$

which manifestly sum to zero as they should. This result is unfortunately but unavoidably more complicated than the corresponding result for $\mathbf{B} = 0$ [17,23,24]. In particular, it requires the computation of $N+1$ inverse tensors, namely, the A_i^{-1} for all *i* (which then determine the D_i and M_i) and M_0^{-1} . However, these inverse tensors can again be analytically evaluated in the usual way [6]. When $\mathbf{B} = \mathbf{0}$, $A_i = \alpha_i$, $M_i = M_0 = U$, and Eq. (39) reduces to its previous simpler form $[17,23]$.

We now return to the question of how to approximate the W_i . In the absence of **B**, where the W_i reduce to scalars w_i , it has been shown [24] that the approximation $w_i = w_0 \rho_i / \sqrt{m_i}$ (where w_0 is a proportionality constant independent of *i*) produces significantly more accurate diffusion fluxes than the obvious simple alternatives $w_i = w_0 \rho_i$ or $w_i = w_0 \rho_i / m_i$. Since motions parallel to **B** are equivalent to motions in $B=0$, we shall accordingly adopt the approximation $w_i^{\parallel} = w_0^{\parallel} \rho_i / \sqrt{m_i}$. Moreover, α_i^{\parallel} and α_i^{\perp} are of the same order of magnitude $[10]$, so it seems reasonable, in the absence of other information, to approximate w_i^{\perp} in the same

form; i.e., $w_i^{\perp} = w_0^{\perp} \rho_i / \sqrt{m_i}$. The proportionality constants w_0^{\parallel} and w_0^{\perp} will of course be different, since $\alpha_i^{\parallel} \neq \alpha_i^{\perp}$ in general. This is immaterial, however, since these constants cancel out in evaluating Ω_i and therefore need not be determined or specified. Indeed, we readily find that

$$
\frac{w_i^{\parallel}}{w^{\parallel}} = \frac{w_i^{\perp}}{w^{\perp}} = \frac{\rho_i / \sqrt{m_i}}{\sum_j \rho_j / \sqrt{m_j}}
$$
(41)

so that

$$
\Omega_i^{\parallel} = \Omega_i^{\perp} = 1 - \frac{\rho_i / \sqrt{m_i}}{\sum_j \rho_j / \sqrt{m_j}} = \Omega_i.
$$
 (42)

Equation (32) then reduces to $\Omega_i = \Omega_i U$, and Eq. (36) reduces to $D_i = p_i \Omega_i A_i^{-1}$.

V. THE LIMIT OF SMALL ELECTRON MASS

The electron mass m_e is very small compared to the masses of the heavy particles, a fact that may be exploited to simplify the preceding general relations. This will be done by neglecting terms of order $\varepsilon \equiv \sqrt{m_e}$ in comparison to terms of order unity. Since the electrical resistivity of the plasma is itself of order ε [6,26], these simplifications will result in an ideal MHD description in which resistive effects vanish. (In the present context, however, the term ''ideal'' does *not* imply that the plasma flow as a whole is isentropic. Diffusion of heavy species, as well as finite-rate chemical reactions, are still irreversible processes.)

A. The Stefan-Maxwell equations and binary diffusion tensors

We begin by observing that α_{ie} is of order ε [13,17–19]. Equation (8) for $i \neq e$ can therefore be rewritten as

$$
\sum_{j \neq e} \alpha_{ij} \cdot (\mathbf{u}_j - \mathbf{u}_i) + \frac{\rho_i q_i}{c} \mathbf{u}_i \times \mathbf{B} = \mathbf{G}_i \quad (i \neq e), \qquad (43)
$$

while the same equation for $i = e$ reduces to

$$
\mathbf{E} = \mathbf{E}_0 - \frac{1}{c} \mathbf{u}_e \times \mathbf{B},\tag{44}
$$

where $\mathbf{E}_0 \equiv (\rho_e q_e)^{-1} (\nabla p_e - \gamma_e)$, and terms proportional to y_e have been neglected since y_e is of order ε^2 . We observe that Eq. (44) is essentially equivalent to the $\sigma \rightarrow \infty$ limit of Eq. (9.47) of Ref. $[26]$, which confirms that we have indeed passed into the realm of ideal MHD. Equation (44) is an explicit expression for **E**, which may be used to eliminate **E** from the \mathbf{G}_i in Eqs. (43). Combining Eqs. (9), (43), and (44) , we obtain

$$
\sum_{j \neq e} \alpha_{ij} \cdot (\mathbf{u}_j - \mathbf{u}_i) + \frac{1}{c} \rho_i q_i (\mathbf{u}_i - \mathbf{u}_e) \times \mathbf{B} = \mathbf{G}_i^0 \quad (i \neq e),
$$
\n(45)

where

$$
\mathbf{G}_{i}^{0} = p \nabla z_{i} + (z_{i} - y_{i}) \nabla p + \frac{y_{i}}{c} \mathbf{J}_{q} \times \mathbf{B} - \rho_{i} q_{i} \mathbf{E}_{0} - \gamma_{i}.
$$
 (46)

The electron velocity \mathbf{u}_e can now be eliminated from Eq. (45) by means of the relation

$$
\rho_e q_e \mathbf{u}_e = \mathbf{J}_q - \sum_{j \neq e} \rho_j q_j \mathbf{u}_j. \tag{47}
$$

By introducing a second type of generalized binary diffusivity tensor for the heavy species alone, the elimination of **u***^e* can be performed in such a way that the result again involves only differences between species velocities. To this end, we make use of the neutrality condition to rewrite Eq. (47) in the form

$$
\rho_e q_e(\mathbf{u}_i - \mathbf{u}_e) = \sum_{j \neq e} \rho_j q_j(\mathbf{u}_j - \mathbf{u}_i) - \mathbf{J}_q, \tag{48}
$$

which combines with Eq. (45) to yield

$$
\sum_{j \neq e} \boldsymbol{\alpha}_{ij}^{\dagger} \cdot (\mathbf{u}_j - \mathbf{u}_i) = \mathbf{G}_i^0 + \frac{\rho_i q_i}{\rho_e q_e c} \mathbf{J}_q \times \mathbf{B} \quad (i \neq e), \quad (49)
$$

where

$$
\boldsymbol{\alpha}_{ij}^{\dagger} = \boldsymbol{\alpha}_{ij} - \frac{\rho_i \rho_j q_i q_j}{\rho_e q_e c} \mathbf{B}. \tag{50}
$$

Note that $\mathbf{a}_{ji}^{\dagger} = \mathbf{a}_{ij}^{\dagger}$ by construction.

Equation (49) now constitutes a system of $N-1$ equations in the $N-1$ unknowns \mathbf{u}_i for $i \neq e$. Only $N-2$ of these equations are linearly independent, however, since their sum over $i \neq e$ yields $\mathbf{0} = \mathbf{0}$. The additional equation needed to close the system is again just the constraint imposed by the given value of the mass-weighted velocity **u**, from which the term y_e **u**_e may be omitted since y_e is of order ε^2 . Once the **u**_{*i*} have been determined for $i \neq e$, \mathbf{u}_e is obtained from Eq. (47).

B. The SCEBD approximation

The central issue here is the order of magnitude of D_e as given by Eq. (36), with Ω_e given by Eq. (42). The deviation of Ω _e from unity is of order ε and may therefore be neglected, whereupon D*^e* simplifies to

$$
D_e = p_e \left(\alpha_e + \frac{\rho_e q_e}{c} B \right)^{-1}
$$

= $p_e \left[\alpha_e^{\parallel} b b + \alpha_e^{\perp} (U - b b) + \frac{\rho_e q_e}{c} B \right]^{-1}$, (51)

in which α_e^{\parallel} and α_e^{\perp} are both of order ε . The tensor inverse can then be evaluated in the usual way $[6]$. When this is done, we find that D_e is of order ε^{-1} , so that $\rho_e D_e$ is of order ε . The $j = e$ term may therefore be omitted from the summation in Eq. (40) for $i \neq e$, which then involves only the D_i for $j \neq e$. The latter in turn involve the α_i for $i \neq e$, which are still given by Eq. (20) . But the $j = e$ term in the summation in Eq. (20) may also be omitted for $i \neq e$, since α_{ie} is of order ε . The α_{i} then no longer appear anywhere in the equations. Finally, once the J_i for $i \neq e$ have thereby been determined by means of Eq. (40) , the diffusion velocity of the electrons is again obtained from Eq. (47) .

VI. CONCLUDING REMARKS

We have presented a hydrodynamic theory of multicomponent diffusion, including thermal diffusion, in twotemperature plasmas in a magnetic field. The theory provides explicit relations that determine the species diffusion fluxes J_i in the plasma. These constitutive relations are an essential ingredient in the multicomponent MHD equations, which otherwise would not in general be closed. The species diffusion fluxes are determined in general by the generalized SM equations (8) or (18) , and in the SCEBD approximation by Eqs. (39) or (40) . In the limit of small electron mass, the SM equations reduce to Eq. (49) , while the SCEBD approximation simplifies as described in Sec. V B. Although the friction and diffusion coefficients in these equations are tensors rather than scalars, the structure of the equations is otherwise similar to that of the equations describing ordinary diffusion in neutral gas mixtures $[17,23,24]$. The present formulation should therefore be equally well suited for practical applications.

As we have seen, the hydrodynamic approach followed here and in Ref. $[17]$ leads naturally to a description of multicomponent diffusion in terms of generalized SM equations. These equations must then be solved or approximated to obtain the species velocities or diffusion fluxes. In contrast, detailed kinetic theories generally lead to explicit formal expressions for the diffusion fluxes in terms of multicomponent $(rather than binary)$ diffusion coefficients $[7-9]$. Thus the latter theories effectively obtain the formal solution of the SM equations during the course of their derivation. However, this apparent advantage is outweighed by the fact that the resulting multicomponent diffusion coefficients are complicated functions of mixture composition and are consequently difficult to compute, whereas the binary friction or diffusion coefficients in the SM equations are simpler and more fundamental quantities, which are independent of composition and only involve the species pair in question. These binary coefficients are given by relatively simple expressions $\left[17-19\right]$, which may readily be evaluated. Moreover, the hydrodynamic derivation provides a clear physical interpretation of the structure of the SM equations in terms of pairwise interactions between species. For these reasons, we share the opinion $[8,27]$ that in spite of their implicit nature, the SM equations are actually preferable to formal expressions for the diffusion fluxes in terms of multicomponent diffusion coefficients.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy under DOE Field Office, Idaho Contract No. DE-AC07-94ID13223, supported in part by the Division of Engineering and Geosciences, Office of Basic Energy Sciences, DOE-OER, and in part by the INEL Long-Term Research Initiative in Computational Mechanics.

- [1] J. D. Ramshaw and C. H. Chang, Plasma Chem. Plasma Process. **12**, 299 (1992).
- [2] C. H. Chang and J. D. Ramshaw, Plasma Chem. Plasma Process. **13**, 189 (1993).
- @3# C. H. Chang and J. D. Ramshaw, Phys. Plasmas **1**, 3698 $(1994).$
- [4] J. A. Shercliff, *A Textbook of Magnetohydrodynamics* (Pergamon, Oxford, 1965).
- [5] J. P. Friedberg, Rev. Mod. Phys. **54**, 801 (1982).
- [6] L. C. Woods, *Principles of Magnetoplasma Dynamics* (Oxford University Press, Oxford, 1987).
- @7# J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954).
- [8] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases,* 3rd ed. ~Cambridge University Press, Cambridge, 1970).
- @9# J. H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).
- [10] S. I. Braginskii, *Transport Processes in a Plasma*, Reviews of Plasma Physics Vol. 1, 205 (Consultant's Bureau, New York, 1965).
- [11] R. M. Chmieleski and J. H. Ferziger, Phys. Fluids 10, 364 $(1967).$
- [12] R. S. Devoto, Z. Naturforsch. **24a**, 967 (1969).
- [13] J. M. Burgers, *Flow Equations for Composite Gases* (Academic, New York, 1969).
- [14] U. Daybelge, J. Appl. Phys. 41, 2130 (1970).
- [15] M. Mitchner and C. H. Kruger, Jr., *Partially Ionized Gases* (Wiley-Interscience, New York, 1973).
- [16] B. V. Alexeev, A. Chikhaoui, J. G. Méolans, J. T. Grushin, and L. P. Grushina, Phys. Plasmas 1, 3199 (1994).
- [17] J. D. Ramshaw, J. Non-Equilib. Thermodyn. **18**, 121 (1993).
- [18] J. D. Ramshaw, J. Non-Equilib. Thermodyn. (to be published).
- $[19]$ J. D. Ramshaw (unpublished).
- [20] J. D. Ramshaw and C. H. Chang, Plasma Chem. Plasma Process. **13**, 489 (1993).
- [21] V. E. Golant, A. P. Zhilinsky, and I. E. Sakharov, *Fundamen*tals of Plasma Physics (Wiley, New York, 1980).
- [22] C. H. Kruger and M. Mitchner, Phys. Fluids **10**, 1953 (1967).
- [23] J. D. Ramshaw, J. Non-Equilib. Thermodyn. **15**, 295 (1990).
- [24] J. D. Ramshaw and C. H. Chang, J. Non-Equilib. Thermodyn. (to be published).
- [25] J. D. Ramshaw, Phys. Fluids 22, 1595 (1979).
- [26] L. C. Woods, *An Introduction to the Kinetic Theory of Gases* and Magnetoplasmas (Oxford University Press, Oxford, 1993), p. 197.
- [27] F. A. Williams, *Combustion Theory*, 2nd ed. (Addison-Wesley, Redwood City, CA, 1985), p. 636.