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Short note

On the ambipolar constraint in multi-component diffusion problems

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1. Introduction

The diffusion velocities in multi-component systems such as plasmas are governed by the Stefan–Maxwell equations. As discussed in [1], the mass flux constraint on these diffusion velocities gives rise to a singularity in the resulting set of continuity equations. In ambipolar plasmas, the assumption of zero-current puts an extra constraint on the diffusion velocities. Similar to the mass flux constraint, this constraint introduces a singularity in the set of continuity equations.

In his extensive paper on ambipolar diffusion [2], Giovangigli identifies this singularity and hints at a possible solution. Here, we will work out the details and obtain a regularized (non-singular) form of the ambipolar diffusion matrix. In addition, we will show that with this regularized ambipolar diffusion matrix and the correct discretization scheme, quasi-neutrality will follow from the numerical method; it does not need to be imposed explicitly.

2. Non-singular formulation of the ambipolar constraint

The mass fraction $y_i = \rho_i/\rho$ of a species i follows from the continuity equation:

$$\frac{\partial}{\partial t}(\rho y_i) + \nabla \cdot (\rho \vec{v} y_i) + \nabla \cdot (\rho \vec{v}_i y_i) = S_i, \tag{1}$$

with $\rho_i = n_i m_i$ the mass density of species i with number density n_i and mass m_i, $\rho = \sum_i \rho_i$ the total mass density, $\vec{v}$ the mass averaged bulk velocity, $\vec{v}_i$ the diffusion velocity and S_i the mass production source term. The diffusion velocity is defined as the velocity with respect to the mass averaged velocity:

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$$\vec{v}_i = \vec{u}_i - \vec{v}, \tag{2}$$

where $\vec{u}_i$ is the total velocity of species i. By their definition, the mass fractions are subject to the constraint

$$\sum_i y_i = 1 \tag{3}$$

and the diffusion velocities to the constraint

$$\sum_i y_i\, \vec{v}_i = 0. \tag{4}$$

As shown in [1], straightforward application of this constraint for the velocities gives rise to a degenerate set of continuity equations.

In plasmas, the drift of charged particles in electric fields causes charge separations over a typical length scale of the Debye length λ_D. This charge separation leads to an electric field, which can be calculated with Poisson's equation. In plasma's where λ_D is small, this approach is not very efficient, since it requires excessively fine meshes. In these plasmas, it is more appropriate to consider the electric field in the limit of vanishing Debye length.

In the limit of vanishing Debye length, the plasma becomes quasi-neutral and there is no current. The electric field necessary to maintain this situation is called the ambipolar field $\vec{E}_{\text{amb}}$. The assumption of an ambipolar plasma puts extra constraints on the mass fractions and the diffusion velocities. The quasi-neutrality constraint can be expressed as:

$$\sum_i \frac{q_i y_i}{m_i} = 0, \tag{5}$$

which is the counterpart of (3), but now for charge instead of mass. The zero-current constraint can be written as:

$$\sum_i n_i q_i\, \vec{v}_i = 0, \tag{6}$$

which is the counterpart of (4). Similar to (4), the zero-current constraint causes singular behaviour. This can be demonstrated by considering a steady-state situation. Multiplying all continuity equations with q_i/m_i and summing over all species gives:

$$\sum_i \left(\nabla \cdot \left(\rho \vec{v} \frac{q_i y_i}{m_i} \right) + \nabla \cdot \left(\rho\, \vec{v}_i\, \frac{q_i y_i}{m_i} \right) \right) = \sum_i \frac{q_i S_i}{m_i}. \tag{7}$$

Since no net charge is produced or destroyed in reactions, the sum on the right hand side of this equation is zero. Introducing the 'charge-neutrality species' $\tau = \sum_i q_i y_i / m_i$ and applying constraint (6) gives:

$$\nabla \cdot (\rho \vec{v} \tau) = 0. \tag{8}$$

This expression becomes degenerate for stagnation points, where $\vec{v} = 0$. As in the mass constraint, this degeneracy is due to the lack of dissipative terms, but now for the 'charge-neutrality species' τ. A solution for this singularity is presented in the next section.

2.1. Ambipolar diffusion matrix

The solution for the singularity induced by the zero-current constraint is found in adding dissipative (diffusive) terms to the expressions for the diffusion velocities without changing the solution. First consider the unchanged expressions for the diffusion velocities. The Stefan-Maxwell equations can be written as [1,3]:

$$\widetilde{\mathbf{F}}\mathbf{v} = -\mathbf{d}, \tag{9}$$

with $\widetilde{\mathbf{F}}$ the regularized friction matrix, $\mathbf{v} = (\vec{v}_1, \ldots, \vec{v}_N)^{\mathrm{T}}$ the vector of diffusion velocities and $\mathbf{d} = (\vec{d}_1, \ldots, \vec{d}_N)^{\mathrm{T}}$ the vector of driving forces. In the following analysis, it is useful to split the driving force $\mathbf{d}$ into the drift caused by the ambipolar electric field $\mathbf{z}\vec{E}_{\text{amb}}/p$ and the remaining driving forces $\mathbf{d}^*$:

$$\widetilde{\mathbf{F}}\mathbf{v} = -(\mathbf{d}^* + \mathbf{z}\vec{E}_{\text{amb}}/p), \tag{10}$$

where p is the pressure and $\mathbf{z} = (n_1 q_1, \ldots, n_N q_N)^{\mathrm{T}}$. Introducing $\mathbf{G} = \widetilde{\mathbf{F}}^{-1}$ yields:

$$\mathbf{v} = -\mathbf{G}(\mathbf{d}^* + \mathbf{z}\vec{E}_{\text{amb}}/p). \tag{11}$$

The ambipolar field is still present in this expression for the diffusion velocities, but can be eliminated by applying constraint (6).

When we define the inner product in species space as $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_i a_i b_i$, the zero-current constraint (6) can alternatively be written as: