EQUATIONS OF HYDRODYNAMICS FOR MULTICOMPONENT MIXTURES WITH TRANSPORT COEFFICIENTS IN HIGHER APPROXIMATIONS

A. V. Gens and G. A. Tirskii

In the present paper we derive a set of equations of multicomponent hydrodynamics which can be solved for higher derivatives for any number of approximations in the Chapman-Enskog procedure. In the usual treatment [1-3], when the transport coefficients are calculated in the first approximation, such a set of equations can be obtained with the aid of the Stefan-Maxwell relationships [1, 7, 8]. In this form the set of equations is very convenient for the practical solution of a number of hydrodynamic problems [6-8].

However, it has been shown [3-5] that the transport coefficients of certain gaseous mixtures calculated by the Chapman-Enskog procedure in the first approximation can differ markedly from the values calculated in higher approximations. For example, the transport coefficients of a fully ionized hydrogen plasma calculated in the fourth approximation by the Chapman-Enskog method agree well with the values calculated by Spitzer [3] but differ from the values calculated in the first approximation by more than 50% (except for the shear viscosity).

In calculations of the transport coefficients in higher approximations the Stefan-Maxwell relationships, which close the macroscopic set of equations, cease to be valid, and the expressions for the diffusion fluxes closing the set in these cases make the set inconvenient for the practical solution of hydrodynamical problems. In order to obtain a convenient form of macroscopic equations these expressions for the diffusion fluxes must be replaced by relationships which can be solved for the concentration gradients of the components, i.e., by relationships of Stefan-Maxwell type. In the present paper such relationships will be obtained for a one-temperature chemically reacting gaseous mixture of arbitrary composition with a spherically symmetric potential of intermolecular interaction.

In the usual treatment, the set of equations of hydrodynamics for a multicomponent mixture (see, for example, the book by Hirschfelder et al. [2]) is a set of partial differential equations which cannot be solved for the higher derivatives of the sought functions. Effective methods of solving such sets of equations do not exist at the present time.

In order to write this set in the normal Cauchy form, the expressions for the diffusion fluxes

\[ I_i = \sum_{j=1}^{n} \sum_{p} m_{ij} m_j D_{ij} - D_{ij} V \ln T \]  

must be replaced by expressions which can be solved for the concentration gradients of the components or for the vectors \( d_j \).

The formal solution of set (1) leads to great computational difficulties since the coefficients \( a_{ij} \) and \( c_{ijk} \), proportional, respectively, to the coefficients of multicomponent diffusion and to the coefficients of thermal diffusion, are themselves the solutions of linear algebraic sets of equations.

where the coefficients $\tilde{Q}_{ij}^{mt}$ are functions of temperature and of the composition of the mixture. Expressions for the coefficients $\tilde{Q}_{ij}^{mt}$ are given in [1,2] and it is readily seen that

$$Q_{ij}^{mt} = \tilde{Q}_{ij}^{mt}$$

(4)

In place of the traditional expressions for the diffusion fluxes (1) and the total heat flux (5) (which close the hydrodynamic equations) we propose to use their parametric representation, in which the transport coefficients no longer appear. The diffusion fluxes of the components, the heat flux, and the transport coefficients will be functions of these parameters, the values of which will become known in the course of solving the problem as a whole. The set of hydrodynamic equations can then be solved for higher derivatives.

Parameters $\alpha_{j}^{t}$ we introduce in the following manner:

$$\alpha_{j}^{f} = - \alpha_{j}^{b} \ln T + n \sum_{i=1}^{v} c_{j}^{i} \alpha_{i}^{f}$$

(6)

The coefficients $\alpha_{j}$ and $c_{j}^{hk}$ satisfy the linear algebraic set of equations (2) and (3).

We shall show that the expressions for the diffusion fluxes (1) are equivalent to

$$n_{m} \alpha_{j}^{f} \left( \frac{2kT}{m_{j}} \right)^{\frac{1}{2}} = 2I_{j}$$

(7)

and that the expressions for the total heat flux (5) are equivalent to

$$q = \frac{5}{4} kT \sum_{j=1}^{v} n_{j} \left( \frac{2kT}{m_{j}} \right)^{\frac{1}{2}} \left( \alpha_{j}^{f} - \alpha_{j}^{b} \right)$$

(8)

Finally, we shall write out the linear algebraic set of equations which the vectors $\alpha_{j}^{t}$ must satisfy.

Indeed, multiply (6) by $m_{j} n_{j} (2kT/m_{j})^{1/2}$. Utilizing the expressions for the multicomponent coefficients of diffusion and thermal diffusion cited in [1]

$$D_{ij} = (rn_{i}/2nm_{j}) (2kT/m_{i})^{1/2} \alpha_{i}^{b}$$

(9)

$$D_{j}^{\gamma} = \frac{1}{2} n_{m_{j}} (2kT/m_{j})^{1/2} \alpha_{j}^{b}$$

(10)

we find that for $t = 0$, Eq. (6) coincides with (1).

Take $t = 1$ and multiply (6) by $5/4 n_{j} kT (2kT/m_{j})^{1/2}$. The thermal conductivity $\lambda$ is given in terms of the coefficients $\alpha_{j}$ by

$$\lambda = - \frac{5}{4} k \sum_{j=1}^{v} n_{j} \left( \frac{2kT}{m_{j}} \right)^{\frac{1}{2}} \alpha_{j}$$

(11)