FORMATION OF GAS FLOWS WITH ACCOUNT FOR THE EFFECTS OF HEAT CONDUCTION, VISCOSITY, DIFFUSION, AND CHEMICAL REACTIONS

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In this paper we examine the formation of one-dimensional-nonsteady gas flows with account for the influence of thermal conduction, viscosity, diffusion, and chemical reactions. An analogous problem but without account for the effect of diffusion and chemical reactions was examined in [1].

It is shown that the effect of chemical reactions is not significant for short times—the gas behaves as an incompressible fluid. The results obtained may be used to calculate gas flows with discontinuous initial conditions with subsequent numerical integration of the Navier-Stokes equations.

As examples we consider the flows of binary gas mixtures which arise upon application of thermal flux to the flat end of a moving piston (1) and during the decay of an arbitrary discontinuity (2).

It is assumed that the internal degrees of freedom of the gas molecules are in equilibrium with the translational degrees of freedom.

1. We use the Navier-Stokes equations [2]

\[
\begin{align*}
\rho \frac{d c_i}{dt} + \frac{\partial}{\partial x} (\rho c_i V_i) &= W_i, \\
\frac{d \rho}{dt} + \rho \frac{d v}{dt} &= 0, \\
\frac{d p_{xx}}{dt} + \frac{\partial \rho_{xx}}{\partial x} &= 0, \\
\rho c_i \frac{dT}{dt} &= -\frac{\partial q_x}{\partial x} - \frac{\partial V}{\partial x} + \\
+ \sum_{i=1}^{r} U_i \frac{\partial}{\partial x} (\rho c_i V_i) - \sum_{i=1}^{r} U_i W_i, \\
\end{align*}
\]

and the ideal equation of state

\[ p = \rho T \sum_{i=1}^{r} \frac{c_i}{m_i}. \]

Here \( \rho \) is the gas density, \( c_i \) is the mass concentration of the \( i \)-th component, \( V_i \) is the diffusion velocity of the \( i \)-th component, \( v \) is the velocity of the center of mass, \( p_{xx} \) is the pressure tensor, \( T \) is the gas temperature, \( r \) is the number of gas components, \( c_V \) is the gas specific heat at constant volume, \( q_x \) is the energy flux density, \( W_i \) is the rate of formation per unit volume of the \( i \)-th component as a result of chemical reactions, \( U_i \) is the internal energy per unit mass of the \( i \)-th component, \( m_i \) is the mass of a molecule of the \( i \)-th component, \( p \) is the hydrodynamic pressure, \( k \) is Boltzmann's constant, \( t \) is time, and \( x \) is the space coordinate.

The new variables are introduced

\[ t' = t, \quad \psi = \int_{x_w(t)}^{x} \rho \, dx. \]

Here \( x_w(t) \) in case (1) is the wall coordinate and in case (2) the line coinciding for \( t = 0 \) with the line of discontinuity of the initial conditions, which travels with the velocity of the gas center of mass.

We assume that for \( t = 0 \)

\[ T = T^\pm, \quad v = v^\pm, \quad \rho = \rho^\pm \]

are given and constant.

Here the plus and minus superscripts denote, respectively, the parameters for \( \psi > 0 \) and \( \psi < 0 \).

The initial concentrations \( c_i^\pm \) are found from the relations for chemical equilibrium, which is assumed for \( t = 0 \).

For \( \psi = 0 \) the equalities for the mass, momentum, and energy flux-densities and the temperature [3,4] are satisfied (subscript \( w \) denotes values at the wall).

In case (1)

\[ g_i^+ = 0, \quad (g_i = \rho c_i V_i), \quad p_{xx}^+ = p_{xxw}, \quad v^+ = v_w, \quad q_x^+ = q_xw, \quad T^+=T^w, \]

In case (2)

\[ g_i^+ = g_i^-, \quad p_{xx}^+ = p_{xxw}^-, \quad v^+ = v^-, \quad q_x^+ = q_x^-, \quad T^+ = T^-, \]

and we also assume that \( c_i^+ = c_i^- \).

The dimensionless variables and functions are introduced (denoted by an overscore)

\[ \tilde{\psi} = \frac{\psi}{T^w}, \quad \tilde{t} = \frac{1}{\mu^w \rho^w \rho_k}, \quad \tilde{\xi} = \frac{\rho_k}{\mu_k \rho_k T^w}, \quad \tilde{v} = \frac{v}{m_i}, \quad \tilde{T} = T^w, \quad \tilde{p} = p \frac{m_i}{\rho_k T^w}. \]

Here \( \mu \) is viscosity, \( \eta \) is shearing viscosity, \( \nu \) is bulk viscosity. System (1.1) in the new variables takes the form (henceforth the overscores are dropped)

\[ \rho \left( \frac{\partial c_i}{\partial \tilde{t}} - \frac{z \partial c_i}{\partial \tilde{x}} \right) + 2 \rho \frac{\partial}{\partial \tilde{z}} g_i = 2 \tau W_i, \]

\[ \frac{\partial p}{\partial \tilde{t}} - \frac{z \partial p}{\partial \tilde{x}} + 2 \rho \frac{\partial v}{\partial \tilde{z}} = 0, \]

\[ \frac{\partial v}{\partial \tilde{t}} - \frac{z \partial v}{\partial \tilde{x}} - 2 \frac{\partial p_{xx}}{\partial \tilde{z}} = 0, \]

\[ \rho c_i \left( \frac{\partial T}{\partial \tilde{t}} - \frac{z \partial T}{\partial \tilde{x}} \right) + 2 \frac{\partial q_x}{\partial \tilde{z}} + \\
+ 2 p_{xx} \frac{\partial v}{\partial \tilde{z}} + 2 \tau \sum_{i=1}^{r} U_i W_i - 2 \rho \sum_{i=1}^{r} U_i \frac{\partial g_i}{\partial \tilde{z}} = 0. \]

In the case of a binary mixture consisting of atoms and molecules of the \( O \) and \( O_2 \) type, between which the reaction \( 2O = O_2 \) takes place, the expressions for the
mass, momentum, and energy flux-densities have the form [2]
\[ \rho \frac{\partial (1 - c_a)}{\partial z} + ... = 0, \]
where \( \rho \) is the density, \( c_a \) is the mass fraction of the atomic component, and \( \frac{\partial}{\partial z} \) is the spatial derivative.

The equation of state has the form
\[ p = \rho \frac{\mu}{\rho D} \left(1 - c_a\right). \]

Here the subscripts \( a \) and \( m \) denote, respectively, the atomic and molecular component, \( \mu \) is the Schmidt number, \( D \) is the binary diffusion coefficient, \( \rho \) is the density, \( c_a \) is the mass fraction of the atomic component.

For small times we seek the functions \( p, c_i, v, T \) in the form of series
\[ f = \sum_{n=0}^\infty f_n(z) \tau^n. \]

We represent \( \mu, p, S, k, \) and \( T \) in the form of series
\[ f = \sum_{n=0}^\infty f_n(z) \tau^n. \]

The boundary conditions for \( z \to \infty \) will be
\[ \frac{\partial}{\partial z} \left( z^n p \right) = 0, \]
\[ \frac{\partial}{\partial z} \left( z^n \rho \right) = 0, \]
\[ \frac{\partial}{\partial z} \left( z^n c_i \right) = 0, \]
\[ \frac{\partial}{\partial z} \left( z^n T \right) = 0. \]

For \( z = 0 \) we have in case (1) from (1.2)
\[ \hat{g}_1 = 0, \]
\[ \hat{p}_{xx} = \hat{p}_{xxn}, \]
\[ \hat{v}_n = \hat{v}_n, \]
\[ \hat{q}_{xn} = \hat{q}_{xn}, \]
\[ \hat{T}_n = \hat{T}_w. \]

Here it is assumed that the piston velocity \( v_w \) and its temperature \( T_w \) may be represented in the form
\[ f_w = \sum_{n=0}^\infty f_{wn} \tau^n. \]

In case (2) we have from (1.3)
\[ \hat{g}_1 = \hat{g}_1, \]
\[ \hat{p}_{xx} = \hat{p}_{xxn}, \]
\[ \hat{v}_n = \hat{v}_n, \]
\[ \hat{q}_{xn} = \hat{q}_{xn}, \]
\[ \hat{T}_n = \hat{T}_n, \]
\[ \hat{c}_n = \hat{c}_n. \]

There are no terms in (2.1)-(2.5) which account for chemical reactions, i.e., for small times the chemical reactions have no effect on the solution.

For the binary mixture the expressions for the fluxes after expansion into a series have the form
\[ \frac{\partial}{\partial z} \left( \rho c_i \right) = 0, \]
\[ \frac{\partial}{\partial z} \left( \rho v_i \right) = 0, \]
\[ \frac{\partial}{\partial z} \left( \rho T \right) = 0. \]

For small deviations from the initial conditions and for small times we write the unknown functions in the form
\[ f = f + \sum_{n=0}^\infty f_n(z) \tau^n. \]

Here \( f \) is the value for \( t = 0 \).

Then in the case of the \( r \)-th component of the mixture in the zeroth approximation we obtain the system of linear differential equations
\[ \sum_{j=1}^{r-1} A_{ij} c_i^j + A_{i0} T_d = \frac{1}{2} z c_i^j, \]
\[ \rho = 0, \]
\[ B_{ij} v_i^j + \frac{1}{2} \rho \tau \]
\[ \sum_{j=1}^{r-1} K_{ij} v_i^j + K_{i0} T_d = \frac{1}{2} z T_d. \]