On a model for multicomponent chemically reacting mixture of viscous fluids

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Abstract. We present results on the existence of globally defined strong generalized solutions for initial boundary value problem which describes motion of a binary chemically reacting mixture of compressible viscous fluids.

1. Introduction

Many technological processes (fuel combustion, crystal growth) take place with the participation of multicomponent chemically active flows. Modeling, for example, pollutant formation, laminar flame extinction, or gas dissociation requires us to take into account complex chemistry mechanisms and transport phenomena. There is, thus, a strong motivation for investigating the equations governing multicomponent chemically active flows and analyzing their mathematical structure and properties.

The full Navier–Stokes–Fourier system supplemented by the reaction-diffusion equations is generally used to describe the flow of a chemically reacting mixture of compressible viscous fluids (gases) [1-3]. These equations express the physical laws of conservation of mass, momentum, total energy of the mixture, and the mass balance of the components.

Certain results on the properties of mathematical models of such mixtures are presented in [4,5] and relate mainly to the sequential stability of weak solutions.

In this paper we consider a system of equations for a binary chemically reacting mixture of viscous compressible fluids in the case of two-dimensional motion [1,2]:

$\partial_t \rho + \text{div}(\rho \vec{u}) = 0,$

$\partial_t (\rho \vec{u}) + \text{div}(\rho \vec{u} \otimes \vec{u}) + \nabla \pi - \text{div} S = 0,$

$\partial_t (\rho c) + \text{div}(\rho c \vec{u}) + \text{div} F = \rho \omega.$

Here $\rho = \rho_1 + \rho_2$ respectively the density of the mixture and density of components; $c = \frac{\rho_1}{\rho_2}$ is the mass concentration of the first components; $\pi = \pi(\rho c)$, the pressure of the mixture, which is present in the form

$\pi = \pi_c(\rho) + \pi_m(\rho, c),$
Let
\[ \pi_c(\rho) = \rho^\gamma, \quad \gamma > 1. \]  
(5)

The component \( \pi_m = \pi_m(\rho, c) \) is the classical molecular pressure of the mixture, which is determined through the Boyle law as a sum of partial pressures \( p_k \):
\[ \pi_m(\rho, c) = \sum_k p_k = \rho \left( \sum_k \frac{c_k}{m_k} \right) = (\alpha_1 c + \alpha_2)\rho, \quad \alpha_1 = \frac{1}{m_1} - \frac{1}{m_2}, \quad \alpha_2 = \frac{1}{m_2}. \]  
(6)

The following formula is also used instead of (6)
\[ \pi_m(\rho, c) = \alpha_2 \rho + \alpha_1 (\rho c)^{\gamma_1}, \quad \gamma_1 > 1. \]  
(7)

The velocity field of the mixture \( \vec{u} = (u, v) \) with the components \( u \) and \( v \) defined as the average mass velocity of the mixture i.e.
\[ \rho \vec{u} = \rho_1 \vec{u}^{(1)}(i) + \rho_2 \vec{u}^{(2)}, \]
where \( \vec{u}^{(i)} \) is the particle velocity of the \( i \)-th component.

The viscous part of the stress tensor \( \mathbf{S} \) obeys the Newton rheological law, namely
\[ \mathbf{S} = 2\mu \mathbf{D}(\vec{u}) + \lambda \text{div}(\vec{u}) \cdot \mathbf{I}, \]  
(8)

where \( \mathbf{D}(\vec{u}) = \frac{1}{2} \left( \nabla \vec{u} + (\nabla \vec{u})^T \right) \), \( \mathbf{I} \) is the identity tensor; coefficients \( \mu \) and \( \lambda \) are the coefficients of dynamic (shear) and volumetric viscosity are generally functions of thermodynamic variables satisfying the following conditions
\[ \mu > 0, \quad 2\mu + 3\lambda \geq 0. \]  
(9)

These inequalities are the consequence of the second law of thermodynamics. It implies, in particular, that the production of entropy associated with the flow of viscous fluid must not be negative.

The diffusion flux \( \vec{F}(\rho, c) \) is determined by the formula [2]
\[ \vec{F} = -\varphi \nabla (\rho c), \quad \varphi > 0. \]  
(10)

The chemical source \( \omega = \omega(c) \) is also termed the species production rates. It is given function of concentration.

All physical characteristics of the flow are functions of coordinates \( (x, y) \) of the flow region points and time \( t \).

There are reasons [5,6], indicating the need for additional requirements for the growth of viscosity and pressure coefficients as functions of density in order to obtain the existence "in general" of strong generalized and classical solutions of the initial boundary value problem for the Navier-Stokes equations of a viscous compressible fluid. Possible variants of such requirements for viscosity coefficients are indicated in [4,5,7], and the approach proposed in [7] served as the basis for the conclusion of new a priori estimates that ensure the existence "as a whole" of strong generalized solutions for the system of equations (1)-(10).

We will consider the functions \( \lambda(\rho), \mu(\rho), \varphi(\rho), \omega(c) \) defined on \([0, +\infty)\) and \([0, 1]\) respectively and satisfying the conditions:
\[ \mu(\rho) = \text{const} > 0, \quad \lambda(\rho) = \rho^\beta, \quad \beta > 3, \]
\[ \varphi = \text{const} > 0, \quad \omega(c) = -\omega_0 c, \quad \omega_0 = \text{const} > 0. \]  
(11)

Suppose also that the flow region is a rectangle
\[ \Omega = \left\{ (x, y) \in \mathbb{R}^2 : 0 < x < 1, \quad 0 < y < 1 \right\}. \]

Let \( T \) is an arbitrary positive number. We introduce the notation \( Q_t = \Omega \times (0, t) \), for \( t \in (0, T] \). We denote the closures of the corresponding sets as \( \bar{\Omega}, \bar{Q}_t \).
2. Statement of the problem and main results
The distribution of velocity \( \vec{u} \), density \( \rho \) and concentration \( c \) are given at the initial time:

\[
\vec{u}|_{t=0} = \vec{u}_0(x,y), \quad \rho|_{t=0} = \rho_0(x,y), \quad c|_{t=0} = c_0(x,y), \quad (x,y) \in \bar{\Omega};
\]

moreover, the initial density and concentration satisfy the inequalities:

\[
0 < m_0 \leq \rho_0(x,y) \leq M_0 < +\infty, \quad 0 < k_0 \leq c_0(x,y) \leq K_0 < 1, \quad (x,y) \in \bar{\Omega},
\]

where \( m_0, M_0, k_0, K_0 \) are some constants.

At the boundary of the flow region, the normal component of the velocity vector and the vorticity are given

\[
\vec{u} \cdot \vec{n}|_{\partial \Omega} = 0, \quad t \in [0,T],
\]

and the impermeability condition of the boundaries for one of the components

\[
\nabla (\rho c) \cdot \vec{n}|_{\partial \Omega} = 0, \quad t \in [0,T].
\]

A strong generalized solution of the problem (1)-(15) means a generalized solution, all derivatives of which involved in (1) - (3) are regular generalized functions and equations (1) - (3) hold almost everywhere in \( Q_T \).

The main result of the paper is the following theorem.

**Theorem.** If the initial data \( \vec{u}_0, \rho_0, \sigma_0 = \rho_0 c_0 \) are such that

\[
\vec{u}_0 \in W^2_2(\Omega), \quad \rho_0 \in W^1_q(\Omega), q > 2, \quad \sigma_0 \in W^2_2(\Omega),
\]

and the fitting condition of the first order are fulfilled

\[
\vec{u}_0 \cdot \vec{n}|_{\partial \Omega} = 0, \quad \text{rot} \vec{u}_0|_{\partial \Omega} = 0, \quad \nabla \sigma_0 \cdot \vec{n}|_{\partial \Omega} = 0,
\]

then there exists a unique strong generalized solution of the problem (1)-(15) in \( Q_T \) satisfying the conditions

\[
\vec{u} \in W^2_1(Q_T), \quad \rho \in W^{1,1}_q(Q_T), \quad \sigma \in W^{2,1}_q(Q_T),
\]

and there are constants \( m_1, M_1, k_1, K_1 \) such that

\[
0 < m_1 \leq \rho \leq M_1 < +\infty, \quad 0 < k_1 \leq c \leq K_1 < 1 \quad \text{in} \quad Q_T.
\]

We briefly describe the scheme of the proof of theorem.

The existence and uniqueness of classical and strong generalized solutions for a sufficiently small period of time is obtained on the basis of [7,8]. Therefore, the main task in the study of the problem "as a whole" is to derive a priori estimates, the constants of which depend only on the data of the problem, but do not depend on the period of existence of the local solution. Then the local solution can be continued for the whole period \([0, T]\). The existence of strong generalized solutions is established by a limit passages in a sequence of smooth solutions corresponding to the smoothed initial data.

The first a priori estimate for the velocity and concentration of the mixture follows from the following identity, which is a mathematical expression of the energy balance

\[
\frac{d}{dt} E[\rho, \vec{u}, c] + D[\vec{u}] + \int_{\Omega} \varphi \gamma_1 (\rho c)^{\gamma_1 - 2} |\nabla (\rho c)|^2 d\Omega + \frac{\gamma_1}{\gamma_1 - 1} \int_{\Omega} (\rho c)^{\gamma_1} d\Omega = 0.
\]
The total energy is determined by the formula

\[ E[\rho, \vec{u}, c] = K[\rho, \vec{u}] + \Pi_1[\rho] + \Pi_2[\rho, c], \]

where \( K[\rho, \vec{u}] = \frac{1}{2} \int_\Omega \rho |\vec{u}|^2 d\Omega \) is the kinetic energy of the mixture and the summands \( \Pi_1 \) and \( \Pi_2 \) have the form

\[ \Pi_1[\rho] = \int_\Omega \frac{\gamma}{\gamma - 1} \rho^\gamma, \]

\[ \Pi_2[\rho, c] = \int_\Omega \alpha_2 \rho \ln \rho d\Omega + \int_\Omega \alpha_1 \frac{(\rho c)^{\gamma_1}}{\gamma_1 - 1} d\Omega. \]

The sum \( \Pi_1[\rho] + \Pi_2[\rho, c] \) specify the potential energy due to the barotropic component of the pressure and chemical reactions. The value \( D = D[\vec{u}] = \int_\Omega \left[ \mu (\text{rot} \vec{u})^2 + (\lambda + 2\mu) (\text{div} \vec{u})^2 \right] d\Omega \)

characterizes the rate of energy dissipation.

The next step of the proof contains the derivation of the norm estimates for the density function \( \rho \) in \( L_p \):

\[ \|\rho\|_{L_p(\Omega)} \leq C \cdot p^{\frac{2}{p-1}}, \quad (16) \]

where \( C \) is a constant determined by the problem data and independent of the number \( p \). Estimates (16) are obtained by involving a following system

\[ \frac{\partial b_1}{\partial t} + u \frac{\partial b_1}{\partial x} + v \frac{\partial b_1}{\partial y} + L = (\lambda + 2\mu) \text{div} \vec{s}, \]

\[ \frac{\partial b_2}{\partial t} + u \frac{\partial b_2}{\partial x} + v \frac{\partial b_2}{\partial y} + b_2 \text{div} \vec{u} = -\mu \text{rot} \vec{u}. \]

Here \( b_1 = (\lambda + 2\mu) \text{div} \vec{u} - \pi, \quad b_2 = -\mu \text{rot} \vec{u}; \]

\[ L = -(\lambda + 2\mu) A \text{div} \vec{u} + (\lambda + 2\mu) B [\text{div}(\alpha \nabla (\rho c)) + \rho w] + (\lambda + 2\mu) \left( u_x^2 + 2u_y \cdot v_x + v_y^2 \right); \]

\[ \vec{s} = (s_1, s_2), \quad s_1 = \frac{1}{\rho} \left( \frac{\partial b_1}{\partial x} + \frac{\partial b_2}{\partial y} \right), \quad s_2 = -\frac{1}{\rho} \left( \frac{\partial b_2}{\partial x} - \frac{\partial b_1}{\partial y} \right); \]

\[ A = \rho \frac{\partial}{\partial \rho} \left( \frac{\pi}{\lambda + 2\mu} \right) + \rho b_1 \frac{\partial}{\partial \rho} \left( \frac{1}{\lambda + 2\mu} \right) + \alpha_1 \gamma_1 \frac{(\rho c)^{\gamma_1}}{\lambda + 2\mu}; \]

\[ B = \alpha_1 \gamma_1 \frac{(\rho c)^{\gamma_1 - 1}}{\lambda + 2\mu}. \]

Estimates of higher order derivatives of the velocity vector and derivatives of the functions \( \rho \) and \( c \) are also based on the use of higher order derivatives of differential equations systems.
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