AN EXACT SOLUTION OF THE NAVIER–STOKES EQUATIONS FOR A CHEMICALLY REACTING MIXTURE OF GASES

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An exact solution of the Navier–Stokes equations is presented for the flow of a viscous heat-conducting chemically reacting mixture of gases in a two-dimensional expanding channel. The conditions for the existence of an exact solution of the source type are: the chemical reactions must be equimolecular in an equilibrium mixture of gases, and they must be second order forward and backward in a nonequilibrium mixture. Numerical results are obtained for the flow of a four-component equilibrium mixture of gases in a two-dimensional nozzle for various Mach numbers (M) and Reynolds numbers (Re).

1. The existence of an exact solution of the Navier–Stokes equations for the internal flow of a viscous compressible gas was first established by Williams [1]. His exact solution describes gas flow in a conical nozzle with a special heat- and mass-transfer law. Byrkin [2] generalized the Hamel solution to the flow of a viscous compressible gas. Shchennikov [3] constructed a class of exact solutions of the Navier–Stokes equations which includes the results of [1, 2] as special cases.

The procedure described in [3] can be generalized to the flow of a chemically reacting mixture of gases.

We consider two-dimensional flows of an m-component chemically reacting mixture of gases consisting of ν chemical elements.

The system of equations describing the flow can be written in the following vector form:

the equations of motion

$$\rho\,(\mathbf{V}\cdot\nabla)\,\mathbf{V} = -\nabla p + {}^{1}\!/_{3}\,\nabla\,(\mu\,\nabla\,\mathbf{V}) + \mu\,\Delta\,\mathbf{V} + \nabla\,(\nabla\mu\cdot\mathbf{V}) - \nabla\times(\nabla\mu\times\mathbf{V}) - \mathbf{V}\,\Delta\mu$$

the equation of continuity

$$\nabla\,(\rho\mathbf{V}) = 0$$

the equation of conservation of energy

$$\rho\mathbf{V}\cdot\nabla\sum_{\alpha=1}^{m} c_\alpha h_\alpha - (\mathbf{V}\cdot\nabla)\,p = \nabla\,(\lambda\nabla T) - {}^{2}\!/_{3}\mu\,(\nabla\mathbf{V})^2 + \mu_\Delta\,(\mathbf{V})^2 -$$

$$-2\mu\mathbf{V}\cdot\nabla(\nabla\mathbf{V}) + 2\mu\Delta\mathbf{V}\times(\nabla\times\mathbf{V}) - \mu\,(\nabla\times\mathbf{V})^2 - \sum_{\alpha=1}^{m}\Delta\,(\mathbf{J}_\alpha h_\alpha)$$

the equations of conservation of chemical elements

$$\sum_{\alpha=1}^{m} n_{\tau\alpha}\nabla\,(\mu c_\alpha\mathbf{V} + \mathbf{J}_\alpha) = 0 \quad (\tau = 1, 2, \ldots, \nu - 1)$$

$$\sum_{\alpha=1}^{m} c_\alpha = 1$$

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the equations of chemical equilibrium for an equilibrium mixture

$$K_{p\beta} = p^{a} \prod_{\alpha=1}^{m} \bar{c}_{\alpha}{}^{b} \quad (\beta = 1, 2, \ldots, m - \nu)$$

$$b = \nu''_{\alpha\beta} - \nu'_{\alpha\beta}, \quad a = \sum_{\alpha=1}^{m} b$$

For a nonequilibrium mixture of gases, m − ν equilibrium equations are replaced by m − ν equations for the diffusion of the chemical components [4].

$$\nabla(\rho\bar{c}_{\alpha}\mathbf{V} + \bar{\mathbf{J}}_{\alpha}) = \sum_{\beta=1}^{N} b\Big(K_{f\beta}\rho^{\Omega} \prod_{l=1}^{m} \bar{c}_{l}{}^{\omega} - K_{b\beta}\rho^{s} \prod_{l=1}^{m} \bar{c}_{l}{}^{\sigma}\Big) \quad (\alpha = 1, 2, \ldots, m-\nu)$$

$$\omega = \nu'_{l\beta}, \quad \Omega = \sum_{l=1}^{m} \omega, \quad \sigma = \nu''_{l\beta}, \quad s = \sum_{l=1}^{m} \sigma$$

The Stefan–Maxwell equations are [5]

$$\sum_{\alpha=1,\,\alpha\neq\beta}^{m} \frac{\bar{c}_{\alpha}\bar{c}_{\beta}}{\rho D_{\alpha\beta}}\left(\frac{\mathbf{J}_{\alpha}}{c_{\alpha}} - \frac{\mathbf{J}_{\beta}}{c_{\beta}}\right) = \left(\sum_{\alpha=1}^{m} \bar{c}_{\alpha}\right)^{2} \nabla \sum_{\alpha=1}^{m} \frac{\bar{c}_{\beta}}{\bar{c}_{\alpha}} +$$

$$+ \nabla \ln T \sum_{\alpha=1,\,\alpha\neq\beta}^{m} \frac{\bar{c}_{\alpha}\bar{c}_{\beta}}{\rho D_{\alpha\beta}}\left(\frac{D_{\alpha}{}^{T}}{c_{\alpha}} - \frac{D_{\beta}{}^{T}}{c_{\beta}}\right) \quad (\beta = 1, 2, \ldots, m - 1)$$

$$\sum_{\alpha=1}^{m} \mathbf{J}_{\alpha} = 0$$

The equation of state is

$$p = \rho RT \sum_{\alpha=1}^{m} \bar{c}_{\alpha}$$

Here $\mathbf{V}$, ρ, p, T, μ, and λ are respectively the velocity, density, pressure, temperature, viscosity, and thermal conductivity of the mixture of gases; c_{α}, h_{α}, $D_{\alpha\beta}$, D_{α}^{T}, and J_{α} are respectively the concentration, specific enthalpy, the binary and thermal diffusion coefficients and the diffusion current density for component α; $n_{\tau\alpha}$ is the number of atoms of chemical element τ in component α; $\nu'_{\alpha.\beta}$ ($\nu''_{\alpha\beta}$) are the stoichiometric coefficients of the αth and βth forward (backward) reaction; $K_{p\beta}$ is the equilibrium constant of the βth reaction; $K_{f\beta}$ and $K_{b\alpha}$ are the reaction rates of the βth forward and the αth backward reactions; R is the universal gas constant; ∇ is the Hamilton operator; $\Delta = \nabla^{2}$ is the Laplacian operator; N is the number of nonequilibrium chemical reactions

$$\bar{c}_{\alpha} = c_{\alpha} / M_{\alpha}, \quad \bar{\mathbf{J}}_{\alpha} = \mathbf{J}_{\alpha} / M_{\alpha}$$

M_{α} is the molecular weight of the αth component.

The system of equations is completed by using the thermodynamic relations for the transfer coefficients and writing h_{α}, $K_{p\beta}$, $K_{f\beta}$, and $K_{b\alpha}$ as functions of the temperature.

2. We seek a transformation of coordinates and unknown functions leaving the initial system of equations and the functional relations completing it invariant. We consider a scale transformation

$$x = x^{*}\xi, \quad y = y^{*}\eta$$

$$\varphi = \varphi^{*}\Phi^{\circ} \quad (\varphi = u, v, p, \rho, T, \ldots)$$

Calculation shows that the required transformation has the form

$$\xi = \eta = 1/C, \quad J_{\alpha}{}^{\circ} = \rho^{\circ} = p^{\circ} = C, \quad D_{\alpha\beta}{}^{\circ} = 1/C \tag{2.1}$$

where C is an arbitrary constant.

The following conditions must be satisfied:

for equilibrium chemical reactions

$$a = 0 \tag{2.2}$$

for nonequilibrium chemical reactions

$$\Omega = s = 2 \tag{2.3}$$

Assuming $C \neq 1$, which is the condition that the transformation (2.1) be nontrivial, we obtain

$$\rho x = \rho^* (z), \quad px = p^* (z) \quad J_\alpha x = I_\alpha (z), \quad D_{\alpha\beta}\, p = d_{\alpha\beta} (z) \tag{2.4}$$

where $z = y/x$.

Condition (2.2) is the requirement that the equilibrium chemical reactions be equimolecular, and (2.3) states that in the nonequilibrium case the forward and backward reactions are second order.

Substituting the self-similar solution (2.4) into the equation of continuity we obtain

$$zu (z) = v (z) \tag{2.5}$$

It follows from (2.5) that the solution (2.4) corresponds to flow from a source at the origin.

If we limit our discussion to the flow within a plane dihedral angle and take account of (2.5), the solution (2.4) describes a constant flow rate along the channel. In this case the x axis is the longitudinal coordinate.

It is shown that as in the Hamel solution, the solution found can satisfy the condition of adhesion to the channel walls, and the problem of formulating other boundary conditions is discussed.

3. We change to polar coordinates r, θ. Using (2.4) and (2.5), we seek a solution in the form

$$\begin{gathered}
v_r = w(\theta), \quad p = r^{-1}p^*(\theta), \quad h_\alpha = h_\alpha(\theta) \\
v_\theta \equiv 0, \quad \rho = r^{-1}\rho^*(\theta), \quad c_\alpha = c_\alpha(\theta) \\
T = T(\theta), \quad D_{\alpha\beta} = p^{-1}d_{\alpha\beta}(\theta), \quad \mu = \mu(\theta) \\
D_\alpha{}^T = D_\alpha{}^T(\theta), \quad K_{pl} = K_{pl}(\theta), \quad K_{fi} = K_{fi}(\theta) \\
K_{bi} = K_{bi}(\theta), \quad \lambda = \lambda(\theta), \quad J_{\alpha r} = r^{-1}I_\alpha(\theta), \quad J_{\alpha\theta} \equiv 0 \\
(\alpha, \beta = 1, 2, \ldots, m; \; l = 1, 2, \ldots, m - \nu; \quad i = 1, 2, \ldots, N)
\end{gathered} \tag{3.1}$$

where v_r, $J_{\alpha r}$, v_θ, and $J_{\alpha\theta}$ are respectively the radial and angular components of the velocity and diffusion current density of component α.

The last of Eqs. (3.1) is a consequence of the Stefan–Maxwell relations resolved along the θ direction.

The dimensionless forms of the equations describing self-similar flow in polar coordinates are

the equations of motion

$$p^* \operatorname{Re} + \varkappa M^2 \left[\frac{d}{d\theta}\left(\mu \frac{dw}{d\theta}\right) - \frac{4}{3}\mu w\right] = 0 \tag{3.2}$$

$$\left(\frac{4}{3}\frac{d\mu w}{d\theta} + \mu \frac{dw}{d\theta}\right)\varkappa M^2 - \operatorname{Re}\frac{dp^*}{d\theta} = 0 \tag{3.3}$$

the equation of conservation of energy

$$\frac{d}{d\theta}\left[\mu \frac{c_p}{\Pr}\frac{dT}{d\theta} + \frac{M^2}{2}(\varkappa - 1)\mu \frac{dw^2}{d\theta} - \frac{1}{\mathrm{Sm}}\sum_{\alpha=1}^{m} I_\alpha h_\alpha\right] = 0 \tag{3.4}$$

the equations for the diffusion of chemical elements

$$\sum_{\alpha=1}^{m} n_{\tau\alpha}\frac{dI_\alpha}{d\theta} = 0 \qquad (\tau = 1, 2, \ldots, \nu - 1) \tag{3.5}$$

$$\sum_{\alpha=1}^{m} \frac{dc_\alpha}{d\theta} = 0 \tag{3.6}$$

the Stefan–Maxwell relations

$$\begin{gathered}\sum_{\alpha=1,\,\alpha\neq\beta}^{m} \frac{p^*\bar{c}_\alpha \bar{c}_\beta}{\rho^* d_{\alpha\beta}}\left(\frac{I_\alpha}{c_\alpha} - \frac{I_\beta}{c_\beta}\right) = \left(\sum_{\alpha=1}^{m} \bar{c}_\alpha\right)^2 \sum_{\alpha=1}^{m} \frac{d}{d\theta}\left(\frac{\bar{c}_\beta}{\bar{c}_\alpha}\right) + \\ + \frac{d\ln T}{d\theta} \sum_{\alpha=1,\,\alpha\neq\beta}^{m} \frac{p^*\bar{c}_\alpha \bar{c}_\beta}{\rho^* d_{\alpha\beta}}\left(\frac{D_\alpha{}^T}{c_\alpha} - \frac{D_\beta{}^T}{c_\beta}\right) \qquad (\beta = 1, 2, \ldots, m-1) \\ \sum_{\alpha=1}^{m} I_\alpha = 0\end{gathered} \tag{3.7}$$

the equation of state

$$p^* = \rho^* T \sum_{\alpha=1}^{m} \bar{c}_\alpha \tag{3.8}$$

the equations of chemical equilibrium for an equilibrium mixture

$$\frac{d}{d\theta}(\ln K_{p\beta}) = \sum_{\alpha=1}^{m} (\nu''_{\alpha\beta} - \nu'_{\alpha\beta}) \frac{d}{d\theta}(\ln \bar{c}_\alpha) \qquad (\beta = 1, 2, \ldots, m - \nu) \tag{3.9}$$

the equations for the diffusion of the chemical components for a nonequilibrium mixture

$$\begin{gathered}\frac{d\bar{I}_\alpha}{d\theta} = \mathrm{Re}\,\mathrm{Sm} \sum_{\beta=1}^{N} (\nu''_{\alpha\beta} - \nu'_{\alpha\beta})\left(K_{f\beta} \prod_{l=1}^{m} \bar{c}_l{}^{\omega} - K_{b\beta} \prod_{l=1}^{m} \bar{c}_l{}^{\sigma}\right)(\rho^*)^2 \\ (\alpha = 1, 2, \ldots, m - \nu)\end{gathered} \tag{3.10}$$

In writing the dimensionless equations the reference quantities were chosen as

$$w_0,\ \rho_0^*,\ T_0,\ \mu_0,\ \lambda_0,\ c_{p_0},\ p_0^* = \rho_0^* R T_0 \quad D_{\alpha\beta 0} = (p_0^*)^{-1} d_{\alpha\beta 0}$$

equal to the values of these quantities at $\theta = 0$. Here λ_0, μ_0, and c_{p_0} are respectively the thermal conductivity, viscosity, and specific heat at constant pressure of the mixture of gases

$$\begin{gathered}\mathrm{Re} = \frac{\rho_0^* w_0}{\mu_0}, \quad \mathrm{Pr} = \frac{c_{p_0}\mu_0}{\lambda_0}, \quad \mathrm{Sm} = \frac{\mu_0}{\rho_0^* D_{\alpha\beta 0}}, \\ M^2 = \frac{w_0^2}{\varkappa R T_0} \qquad \left(\varkappa = \frac{c_{p_0}}{c_{v_0}},\ c_{v_0} = c_{p_0} - R\right)\end{gathered}$$

where Re is the Reynolds number, Pr is the Prandtl number for the mixture of gases, Sm is the Schmidt number calculated from one of the characteristic binary diffusion coefficients of the mixture, e.g., the largest, and M is the Mach number.

Let us discuss some general properties of the self-similar solution (3.1).

We add (3.3) to the derivative of (3.2). The solution of the resulting differential equation

$$\frac{d^2}{d\theta^2}\left(\mu \frac{dw}{d\theta}\right) + \mu \frac{dw}{d\theta} = 0$$

is

$$\mu \frac{dw}{d\theta} = A \cos(\theta + \vartheta)$$

where A and ϑ are arbitrary constants.

For symmetric flow within a two-dimensional nozzle, i.e., $dw/d\theta = 0$ at $\theta = 0$, we have by using (3.2)

$$\mu\, dw/d\theta = A \sin\theta$$
$$(A = {}^4/_3 - \mathrm{Re}/(\varkappa M^2))$$

We require that the adhesion condition be satisfied at $\theta = \theta_W$, where θ_W is the half-angle opening of the nozzle, i.e., $w(\theta_W) = 0$. We obtain from (3.2) an expression for the pressure at the nozzle wall,

$$p_w{}^* = p^*(\theta_w) = -(\varkappa M^2/\mathrm{Re})\, A \cos\theta_w$$

from which it follows that

$$\theta_w < \pi/2$$

The adhesion condition at the nozzle wall can be satisfied by taking $A < 0$, i.e., when

$$\mathrm{Re} > {}^4/_3\, \varkappa M^2$$

Integrating (3.4) once and using (3.5) gives

$$\mathrm{Sm}\,\mu \frac{c_p}{\mathrm{Pr}} \frac{dT}{d\theta} + (\varkappa - 1) M^2 A w \sin\theta - \sum_{\alpha=1}^{m} I_\alpha h_\alpha = C^* \tag{3.11}$$

where C^* is an integration constant. For symmetric flow $C^* = 0$. Using $C^* = 0$ it follows from (3.6) that the condition that the walls be noncatalytic $[I_\alpha(\theta_W) = 0,\ \alpha = 1, 2, \ldots, m]$ is satisfied only for adiabatic walls, i.e., when $(dT/d\theta)_W = 0$.

We note another property of the self-similar solutions. It follows from (3.5) that

$$\sum_{\alpha=1}^{m} n_{\tau\alpha} I_\alpha = C_\tau^{**} \quad (\tau = 1, 2, \ldots, \nu - 1) \tag{3.12}$$

where the C_τ^{**} are integration constants. Taking account of the symmetry of the flow conditions we find that $C_\tau^{**} = 0$, i.e., the concentrations of chemical elements remain constant during the flow.

4. Let us consider in more detail a scheme for calculating the symmetric flow of an equilibrium mixture of gases in a two-dimensional nozzle. We start with Eqs. (3.6)-(3.12).

We arbitrarily divide the problem into dynamical and diffusion parts. The first relates to the equations of motion and conservation of energy, and the second to the remaining equations. The condition that the reactions be equimolecular permits a solution of the diffusion part of the problem in the form of concentrations as functions of the temperature. By substituting this solution into the equation for the conservation of energy we seek a solution of the problem as a whole.

We write the solution of the equations for the diffusion part of the problem (3.6)-(3.9), (3.12) in the form of concentration gradients and diffusion current density components as functions of the temperature gradient

$$dc_\alpha/d\theta = f_\alpha(c_1, \ldots, c_m, T)\, dT/d\theta \quad (\alpha = 1, 2, \ldots, m) \tag{4.1}$$

$$I_\alpha = F_\alpha(c_1, \ldots, c_m, T)\, dT/d\theta \quad (\alpha = 1, 2, \ldots, m) \tag{4.2}$$

Using (4.2) we have from (3.11)

$$\frac{dT}{d\theta} = -\frac{\mathrm{Sm}\,\mathrm{Pr}\, M^2(\varkappa - 1) A w \sin\theta}{c_p \mathrm{Sm}\,\mu - \mathrm{Pr} \sum\limits_{\alpha=1}^{m} F_\alpha h_\alpha} \tag{4.3}$$

The problem can be solved numerically by integrating the system of ordinary differential equations (3.10), (3.11), (4.1), and (4.3) by a standard numerical method.

The symmetry of flow conditions for $\theta = 0$

$$\frac{dc_\alpha}{d\theta} = 0 \quad (\alpha = 1, 2, \ldots, m), \qquad \frac{dT}{d\theta} = \frac{dw}{d\theta} = 0$$

and the adhesion condition $w = 0$ at $\theta = \theta_W$ can be used as boundary conditions.

The numerical solution is obtained in the process of integrating the system of equations from $\theta = 0$ to $\theta = \theta_W$, with $w(\theta_W) = 0$. It follows from (4.3) that then $(dT/d\theta)_W = 0$, i.e., the adiabatic condition (noncatalytic walls) is satisfied.

5. As an example we present the results of numerical calculations of the flow of an equilibrium mixture of gases consisting of the four components H_2, H_2O, CO, and CO_2. We assume that the following equimolecular reaction occurs during the flow:

$$H_2O + CO \rightleftarrows CO_2 + H_2$$

The equilibrium constant of this reaction can be written as the ratio of the equilibrium constants of the reactions

$$2H_2O \rightleftarrows 2H_2 + O_2, \quad 2CO + O_2 \rightleftarrows 2CO_2$$

and is related to the concentrations of the chemical components by the following equilibrium equations:

$$K_p = \bar{c}_1\bar{c}_2 / \bar{c}_3\bar{c}_4 \qquad (c_1 = c_{H_2O},\ c_2 = c_{CO},\ c_3 = c_{CO_2},\ c_4 = c_{H_2})$$

The viscosity of the mixture was calculated by formula [6], and the Prandtl number of the mixture is

$$\Pr = c_p / (1.204\, c_p + 1.47)$$

where c_p is the specific heat of the mixture of gases. The specific heats and enthalpies of the components were calculated by using the interpolation formulas given in [7].

Numerical calculations were performed for T(0) = 1700°K and no thermal diffusion. The results of the calculations are shown in Figs. 1-4. Figure 1 shows the reduced temperature profile T/T_p (solid curve), where T_p is the temperature corresponding to the flow of a frozen mixture of gases

$$T_p = (\varkappa - 1) M^2 \Pr (1 - w^2) / 2 c_p + 1$$

and the temperature profile (open curve). The numbers on the curves correspond to flows at various M and Re numbers: 2) M = 2, Re = 100; 3) M = 3, Re = 100; 4) M = 1, Re = 100. For comparison the reduced temperature profile T/T_p is shown for M = 3, Re = 100 and no diffusion (curve 1). Figure 2 shows the temperature

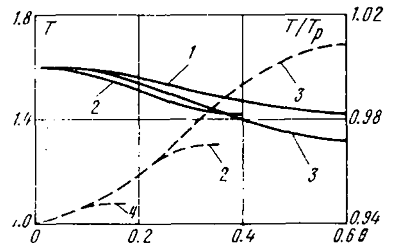

Fig. 1

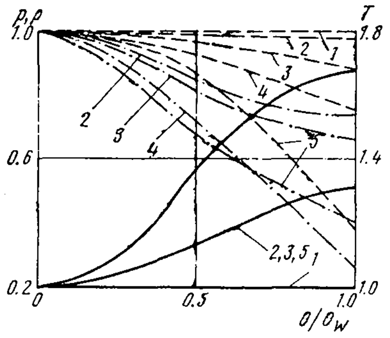

Fig. 2

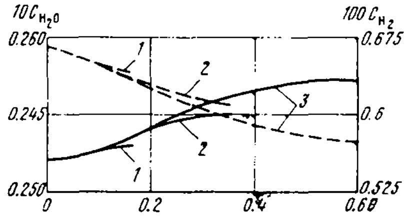

Fig. 3

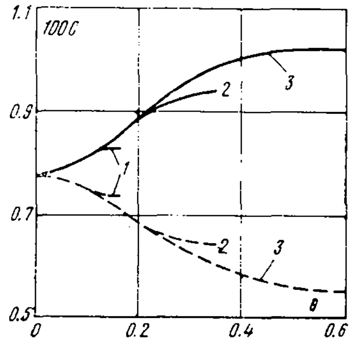

Fig. 4

profile (solid curve), the pressure (dashed curve), and the density (dot-dash curve): 1) M = 0.2, Re = 100; 2) M = 2, Re = 1000; 3) M = 2, Re = 100; 4) M = 3, Re = 100; 5) M = 2, Re = 20.

Figure 3 shows profiles of the reduced concentrations $\bar{c}$ of water vapor (solid curves) and molecular hydrogen (open curves) corresponding to flows with Re = 100 and various M values: 1) M = 1; 2) M = 2; 3) M = 3.

Figure 4 shows profiles of the reduced concentrations of carbon monoxide (solid curves) and carbon dioxide (open curves). The numbers on the curves and the values of the flow parameters are the same as in Fig. 3.

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