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A first-order hyperbolic system of governing equations for miscible and viscous compressible fluids

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Abstract: In this paper we introduce a reformulation of the compressible multicomponent Navier–Stokes equations that govern the behaviour of mixtures of miscible gases. The resulting equation set is a first-order hyperbolic system containing stiff source terms, which recovers the conventional parabolic theory of viscosity, conduction and diffusion as a first-order approximation in the relaxation limit. An important advantage of this approach versus other first-order reformulations of the Navier–Stokes equations is that the wave speeds remain finite as some relaxation parameter tends to zero. The complete system of equations is presented in one-dimension for binary mixtures of viscous, heat conducting gases.

Keywords: Governing Equations, Diffuse Interface, Multispecies.

1 Introduction

This paper is concerned with the modelling and numerical simulation of gaseous mixtures at the continuum level, a topic of great importance in many scientific and engineering disciplines such as astrophysics and combustion [1, 2]. In particular, it is motivated by the desire to conduct direct numerical simulations (DNS) of flows that contain shock waves, material interfaces and fine-scale turbulent structures. This combination of flow features poses significant conflicting requirements on the numerical method that is used, which must be both robust enough to capture the various discontinuities in the flow but still have good fidelity in the high wavenumber range of the flow. In particular for DNS, the numerical method should preferably be high-order accurate in multiple dimensions as this will greatly increase the efficiency of the computation [3]. Numerical methods that satisfy all of these requirements are most easily designed for systems of hyperbolic conservation laws, as the theory of hyperbolic partial differential equations is much more advanced than for more general systems [4]. Thus if the governing equations that describe mixtures of miscible, viscous, compressible fluids can be written as a system of hyperbolic conservation laws, this allows for the straightforward application of modern high-order numerical methods which will in turn enable efficient DNS of these flows to be conducted for higher Reynolds numbers than are currently achievable.

1.1 Conventional governing equations

The conventional mathematical description of these flows is given by the multicomponent Navier-Stokes equations [5], which can be derived from the Boltzmann equation using Chapman-Enskog theory [6]. In general, the molecular transport terms that arise from this derivation cannot be related to the primary flow variables and a further level of approximation is required [7], leading to the classical laws of viscosity, thermal diffusion and multicomponent mass diffusion [8]. The multicomponent Navier-Stokes equations can be written in strong conservation form as follows:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0\\
&\frac{\partial \rho Y_k}{\partial t} + \nabla\cdot(\rho Y_k\boldsymbol{u}) = -\nabla\cdot(\boldsymbol{\mathcal{J}}_k) \qquad k = 1,\ldots,N-1\\
&\frac{\partial \rho\boldsymbol{u}}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}^T + p\boldsymbol{I}) = -\nabla\cdot\boldsymbol{\sigma}\\
&\frac{\partial \rho E}{\partial t} + \nabla\cdot\big([\rho E + p]\boldsymbol{u}\big) = -\nabla\cdot(\boldsymbol{\sigma}\cdot\boldsymbol{u} + \boldsymbol{q})
\end{aligned} \tag{1}$$

In Eqn. (1), ρ is the mass density, Y_k are species mass fractions, $\boldsymbol{u}$ is the mass-weighted velocity, p is the pressure and $E = e + \frac{1}{2}\boldsymbol{u}^2$ is the total energy, where the internal energy e is determined by the equation of state. For a Newtonian fluid the viscous stress tensor $\boldsymbol{\sigma}$ is given by:

$$\boldsymbol{\sigma} = -\eta\big(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\big) + \Big(\frac{2}{3}\eta - \eta_b\Big)\nabla\cdot\boldsymbol{u}\boldsymbol{I} \tag{2}$$

where η is the coefficient of dynamic viscosity and η_b is the coefficient of bulk viscosity, which is typically neglected (since kinetic theory predicts $\eta_b = 0$ for a monatomic gas). The diffusion flux $\boldsymbol{\mathcal{J}}_k$ for species k is given by:

$$\boldsymbol{\mathcal{J}}_k = \rho Y_k \boldsymbol{V}_k \tag{3}$$

where $\boldsymbol{V}_k$ is the diffusion velocity of species k. In the general case these diffusion velocities must be determined by solving a linear system of size N^2 [5], however for binary systems the relationship becomes explicit and $\boldsymbol{\mathcal{J}}_1 = \boldsymbol{\mathcal{J}}$ is given by:

$$\boldsymbol{\mathcal{J}} = -\rho D\Big(\nabla Y_1 + \frac{k_T}{T}\nabla T + \frac{k_p}{p}\nabla p\Big) \tag{4}$$

where D is the coefficient of mass diffusion, $k_T D$ is the coefficient of thermal diffusion and $k_p D$ is the coefficient of baro-diffusion [9]. Similarly, the heat flux $\boldsymbol{q}$ for a binary system is given by:

$$\boldsymbol{q} = \Big(k_T\frac{\partial \mu}{\partial Y_1} - T\frac{\partial \mu}{\partial T} + \mu\Big)\boldsymbol{\mathcal{J}} - \kappa\nabla T \tag{5}$$

where μ is the chemical potential and κ is the thermal conductivity of the mixture. In the absence of diffusion, the heat flux $\boldsymbol{q}$ reduces to Fourier's law of conduction. Typically in binary mixing calculations, baro-diffusion and thermal diffusion terms (and their reciprocal heat fluxes) are ignored, although these effects may be non-negligible if the two fluids have large molecular weight ratios [7]. In this paper they are retained in order to satisfy the second law of thermodynamics when comparing with the diffusion terms in the new model.

1.2 First-order hyperbolic formulation

Recently, a unified first-order hyperbolic formulation of continuum mechanics has been proposed in [10, 11], which is in theory capable of describing the entire spectrum of viscous flows and even elastic and plastic deformations in solids. The main features of this model that are desirable from both a mathematical and physical standpoint are that it is a consistent, overdetermined system that is compatible with the first and second laws of thermodynamics and is symmetric hyperbolic, which implies that it is well-posed and causal [11]. Dissipative processes are modelled as algebraic source terms with a characteristic relaxation time for each process. Since these terms do not depend on any space derivatives, the characteristic speeds of the system remain finite regardless of whatever value the relaxation time takes, unlike other relaxation approaches that are used in hyperbolic reformulations of the Navier-Stokes equations [12, 13]. Through formal asymptotic expansion it can be shown that this purely hyperbolic description of viscous dissipation and thermal conduction includes Newton's law of viscosity and Fourier's law of conduction as a first order approximation in the stiff relaxation limit. The work presented in this paper builds on this model by adding a hyperbolic description of binary diffusion of gaseous mixtures to the existing framework.

A first-order hyperbolic system is also advantageous for various numerical reasons as well, as it will be less sensitive to irregularities in the computational mesh, will allow a higher order of accuracy scheme for a given stencil and will be subject to a less restrictive stability condition ($\mathcal{O}(\Delta x)$ vs. $\mathcal{O}(\Delta x^2)$), therefore allowing a larger time step. In cells where the time step in a conventional Navier-Stokes code would be viscous limited (such as in a boundary layer), the time step in the first-order hyperbolic model would only be subject to a CFL condition, giving a $\mathcal{O}(1/\Delta x)$ speedup in computational efficiency [12]. Hyperbolicity also means that a wide range of numerical methods are available (e.g. finite volume [4], discontinuous Galerkin [14], residual distribution [15], active flux [16]), allowing the use of the best suited numerical method for the problem at hand. Thus methods that were developed for the inviscid part of the Navier-Stokes equations, such as upwind fluxes and limiters, can be directly applied to the entire hyperbolic model, enabling a simple and uniform discretisation.

Given the many advantages outlined above to having a first-order hyperbolic formulation of viscous fluid dynamics, it is therefore of great interest to investigate whether the formulation can be extended to include diffusion in the miscible, multicomponent case. For the sake of simplicity only binary diffusion will be considered here. Given the nature of the model, it is only necessary to consider mass diffusion and heat conduction in the initial formulation, the terms relating to viscosity can be included afterwards for the complete description. The derivation is structured as follows; starting from a master system of generating equations (inspired by a single entropy approximation of the equations governing multiphase flow), source terms are introduced such that the production of entropy is non-negative. Following this, the link with the classical theory of binary diffusion is established by considering the kinetic coefficients of these source terms in the relaxation limit. The derivation is completed by presenting the new system of equations in terms of the parameters of state.

2 Generating system of conservation laws for binary mixtures

In this section a master system for compressible and miscible binary mixtures is formulated, from which the governing equations are generated. The form of the master system is inspired by the equations of multiphase flow, specifically the single entropy approximation presented in [17] where the mixture is characterised by a single entropy s. As in the multicomponent Navier-Stokes equations, both species are assumed to be in pressure and temperature equilibrium. In one dimension, the parameters of state that describe the mixture are:

$$\{\rho, Y_1, u, \tilde{w}, J, s\}$$

The definitions of ρ, Y_1 and u are the same as in the conventional theory, however two new state parameters are introduced to incorporate mass diffusion and heat conduction as per the theory of thermodynamically compatible systems [18]. The thermal impulse J has been introduced previously in [11], while $\tilde{w}$ is an artificial variable (of similar form to the relative velocity w used in multiphase models) that is defined such that its energy gradient in state space, $\frac{\partial E}{\partial \tilde{w}}$, is equal to the diffusion flux $\mathcal{J}$. Assuming that the total energy E is a function of $\rho, Y_1, u, \tilde{w}, J$ and s, the generating system in one dimension is given by:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\Big(\rho u\Big) = 0 \\
&\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x}\Big(\rho Y_1 u + E_{\tilde{w}}\Big) = 0 \\
&\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}\Big(\rho u^2 + \rho^2 E_\rho\Big) = 0 \\
&\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x}\Big(\rho \tilde{w} u + E_{Y_1}\Big) = 0 \\
&\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x}\Big(\rho J u + E_s\Big) = 0 \\
&\frac{\partial \rho s}{\partial t} + \frac{\partial}{\partial x}\Big(\rho s u + E_J\Big) = 0
\end{aligned} \tag{6}$$

where E_ξ denotes the partial derivative $\frac{\partial E}{\partial \xi}$. The fact that the total energy E is not an unknown but rather a potential that depends on the remaining unknowns is an important feature of this system, as it means that solutions of the above system of equations also satisfy the additional conservation law:

$$\frac{\partial \rho E}{\partial t}+\frac{\partial}{\partial x}\Big(\Big[\rho E+p\Big]u+E_{Y_1}E_{\tilde{w}}+E_sE_J\Big)=0 \tag{7}$$

which describes the conservation of total energy (note that $p=\rho^2E_\rho$). The requirement that E is a potential and that all of the constitutive terms in the fluxes (and source terms when they are introduced later) in Equation 6 are generated from this potential means that the overdetermined system 6–7 is consistent [11]. Moreover, if the energy potential is a convex function then Equation 6 can be transformed into a symmetric hyperbolic form (see [17] for details), which implies that it is well-posed.

2.1 Introduction of source terms

Source terms are now introduced into the master system to represent the dissipative processes of diffusion and conduction. This is done with adherence to the following requirements; the total energy conservation law must not be affected, production of entropy must be non-negative and the Onsager principle of symmetric kinetic coefficients is assumed to hold. Taking this into account, the governing equations with dissipation are given by:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}\Big(\rho u\Big)=0\\
&\frac{\partial \rho Y_1}{\partial t}+\frac{\partial}{\partial x}\Big(\rho Y_1u+E_{\tilde{w}}\Big)=0\\
&\frac{\partial \rho u}{\partial t}+\frac{\partial}{\partial x}\Big(\rho u^2+\rho^2E_\rho\Big)=0\\
&\frac{\partial \rho\tilde{w}}{\partial t}+\frac{\partial}{\partial x}\Big(\rho\tilde{w}u+E_{Y_1}\Big)=-\theta_{11}E_{\tilde{w}}-\theta_{12}E_J\\
&\frac{\partial \rho J}{\partial t}+\frac{\partial}{\partial x}\Big(\rho Ju+E_s\Big)=-\theta_{21}E_{\tilde{w}}-\theta_{22}E_J\\
&\frac{\partial \rho s}{\partial t}+\frac{\partial}{\partial x}\Big(\rho su+E_J\Big)=Q
\end{aligned} \tag{8}$$

where $\theta_{ij}\geq 0$ are the kinetic coefficients (note that $\theta_{12}=\theta_{21}$), interpreted here as relaxation parameters where the eigenvalues of the matrix $\boldsymbol{\theta}=[\theta_{ij}]$ characterise the rate of relaxation of the heat flux and species mass flux. The entropy production Q should be non-negative and is derived such that the total energy conservation law remains unchanged. This gives:

$$Q=\frac{1}{E_s}\Big(\theta_{11}E_{\tilde{w}}^2+2\theta_{12}E_{\tilde{w}}E_J+\theta_{22}E_J^2\Big)\geq 0 \tag{9}$$

thus meeting all of the requirements for the introduction of source terms into the master system. Since the energy conservation law has remained unchanged and the production of entropy is non-negative, then the master system with source terms included satisfies both the first and second laws of thermodynamics respectively.

2.2 Closure relations

The remaining task now is to define closure relations for the master system so that the governing equations can be generated. The total energy must be defined such that the governing equations that are generated have physical meaning, and is distributed as follows:

$$E(\rho,Y_1,u,\tilde{w},J,s)=E_1(\rho,Y_1,s)+E_2(\tilde{w},J)+E_3(u) \tag{10}$$

where E_1 is the internal energy, E_2 is the non-equilibrium energy and $E_3=\frac{1}{2}u^2$ is the kinetic energy per unit mass. The internal energy $e=E_1$ is defined as the mass-weighted average of the internal energies of each species, which are defined through an equation of state of the form $\epsilon_k=\epsilon_k(\rho_k,s)$. Therefore:

$$e(\rho,Y_1,s)=Y_1\epsilon_1(\rho_1,s)+Y_2\epsilon_2(\rho_2,s) \tag{11}$$

Note that the partial density $\rho_k = \frac{\rho Y_k}{z_k}$ depends on the volume fraction z_k and thus $e = e(\rho, Y_1, z_1, s)$. However, given the assumption of pressure and temperature equilibrium (i.e $p_1 = p_2$ and $T_1 = T_2$) then z_k can be determined from Y_1 as it will be equivalent with the mole fraction $X_k = \frac{W}{W_k} Y_k$ [19], where W_k is the molecular weight of species k and W is the molecular weight of the mixture. The non-equilibrium energy is defined as:

$$E_2(\tilde{w}, J) = \alpha^2 \frac{J^2}{2} + \beta^2 \frac{\tilde{w}^2}{2} \tag{12}$$

where α and β are parameters yet to be determined. With these definitions, the energy gradients in state space may now be determined. Following [20], they are given by:

$$E_\rho = \frac{z_1 p_1 + z_2 p_2}{\rho^2} = \frac{p}{\rho^2} \qquad E_{Y_1} = \mu_1 - \mu_2 \qquad E_s = T \qquad E_{\tilde{w}} = \beta^2 \tilde{w} \qquad E_J = \alpha^2 J \tag{13}$$

where $\mu_k = \epsilon_k + \frac{p_k}{\rho_k} - sT$ is the chemical potential for species k, meaning that the gradient E_{Y_1} is just the difference in species enthalpies.

3 Determination of kinetic coefficients in the relaxation limit

The introduction of kinetic coefficients into the master system allows for a hyperbolic approximation of the parabolic theory for diffusive heat and mass transfer by considering the stiff relaxation limit i.e. for small relaxation times. In the model thermal and mass diffusion are coupled (due to the $\theta_{12} = \theta_{21}$ coefficient) and therefore an explicit relaxation time for each process cannot be defined, however it is sufficient to consider the eigenvalues of the matrix Θ which characterise the rate of relaxation. These are assumed to be much larger than the characteristic rate of transfer of each process. Therefore in the relaxation limit the time derivative and the convective term in the equations for $\tilde{w}$ and J can be neglected, resulting in:

$$\begin{bmatrix} \theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{bmatrix} \begin{bmatrix} E_{\tilde{w}} \\ E_J \end{bmatrix} = - \begin{bmatrix} \frac{\partial E_{Y_1}}{\partial x} \\ \frac{\partial E_s}{\partial x} \end{bmatrix} \tag{14}$$

Therefore:

$$\begin{aligned} E_{\tilde{w}} &= -\chi_{11} \frac{\partial E_{Y_1}}{\partial x} - \chi_{12} \frac{\partial E_s}{\partial x} \\ E_J &= -\chi_{21} \frac{\partial E_{Y_1}}{\partial x} - \chi_{22} \frac{\partial E_s}{\partial x} \end{aligned} \tag{15}$$

where the matrix $\boldsymbol{\chi} = [\chi_{ij}]$ is given by:

$$\begin{bmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{bmatrix} = \begin{bmatrix} \theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{bmatrix}^{-1} \tag{16}$$

The aim now is to relate the derivatives $E_{\tilde{w}}$ and E_J to the diffusive and thermal fluxes. For conventional parabolic theory these will depend on gradients of Y_1, T and p in the most general case [9], therefore the derivative $\frac{\partial E_{Y_1}}{\partial x}$ is written as follows:

$$\frac{\partial E_{Y_1}}{\partial x} = E_{Y_1 Y_1} \frac{\partial Y_1}{\partial x} + E_{Y_1 T} \frac{\partial T}{\partial x} + E_{Y_1 p} \frac{\partial p}{\partial x} \tag{17}$$

Noting that $E_s = T$, Equation 15 becomes:

$$\begin{aligned} E_{\tilde{w}} &= -\chi_{11} E_{Y_1 Y_1} \frac{\partial Y_1}{\partial x} - \left(\chi_{11} E_{Y_1 T} + \chi_{12}\right) \frac{\partial T}{\partial x} - \chi_{11} E_{Y_1 p} \frac{\partial p}{\partial x} \\ E_J &= -\chi_{21} E_{Y_1 Y_1} \frac{\partial Y_1}{\partial x} - \left(\chi_{21} E_{Y_1 T} + \chi_{22}\right) \frac{\partial T}{\partial x} - \chi_{21} E_{Y_1 p} \frac{\partial p}{\partial x} \end{aligned} \tag{18}$$

These need to be related to the the conventional parabolic description, given by Equations 4 and 5:

$$\begin{aligned}\mathcal{J} &= -\rho D\Big(\frac{\partial Y_1}{\partial x} + \frac{k_T}{T}\frac{\partial T}{\partial x} + \frac{k_p}{p}\frac{\partial p}{\partial x}\Big)\\ q &= \Big(k_T\frac{\partial \mu}{\partial Y_1} - T\frac{\partial \mu}{\partial T} + \mu\Big)\mathcal{J} - \kappa\frac{\partial T}{\partial x}\end{aligned}\tag{19}$$

Now, given that $E_{Y_1} = \mu = \mu_1 - \mu_2 = h_1 - h_2$ where the species enthalpy $h_k = \epsilon_k(\rho_k, s) + \frac{p_k}{\rho_k}$, it can be evaluated as follows:

$$\begin{aligned}\frac{\partial}{\partial x}(h_1 - h_2) &= \Big(\frac{\rho c_1^2}{\rho_1 z_1} + \frac{\rho c_2^2}{\rho_2 z_2}\Big)\frac{\partial Y_1}{\partial x} - \Big(\frac{\rho Y_1 c_1^2}{\rho_1 z_1^2} + \frac{\rho Y_2 c_2^2}{\rho_2 z_2^2}\Big)\frac{\partial z_1}{\partial x} + \Big(\frac{Y_1 c_1^2}{\rho_1 z_1} - \frac{Y_2 c_2^2}{\rho_2 z_2}\Big)\frac{\partial \rho}{\partial x}\\ &= \Big(\frac{c_1^2}{Y_1} + \frac{c_2^2}{Y_2}\Big)\frac{\partial Y_1}{\partial x} - \Big(\frac{c_1^2}{z_1} + \frac{c_2^2}{z_2}\Big)\frac{\partial z_1}{\partial x} + \Big(\frac{c_1^2}{\rho} - \frac{c_2^2}{\rho}\Big)\frac{\partial \rho}{\partial x}\end{aligned}\tag{20}$$

where c_k is the speed of sound in species k, defined as $c_k^2 = \frac{\partial p_k}{\partial \rho_k}$. Using the assumption of pressure and temperature equilibrium, the volume fraction $z_k = \frac{W}{W_k}Y_k$, which gives:

$$\frac{\partial z_1}{\partial x} = \frac{W^2}{W_1 W_2}\frac{\partial Y_1}{\partial x}\tag{21}$$

where W is the mixture molecular weight, defined as:

$$\frac{1}{W} = \sum_k \frac{Y_k}{W_k}\tag{22}$$

Since $\rho = \rho Y_1 + \rho Y_2 = \rho_1 z_1 + \rho_2 z_2$ then the derivative $\frac{\partial \rho}{\partial x}$ can be written as:

$$\frac{\partial \rho}{\partial x} = (\rho_1 - \rho_2)\frac{\partial z_1}{\partial x} + z_1\frac{\partial \rho_1}{\partial x} + z_2\frac{\partial \rho_2}{\partial x}\tag{23}$$

To evaluate the derivative $\frac{\partial \rho_k}{\partial x}$ an equation of state must be defined for each species. Assuming both gases are ideal gives:

$$\rho_k = \frac{PW_k}{\mathcal{R}T}\tag{24}$$

where $\mathcal{R}$ is the universal gas constant. Thus $\frac{\partial \rho_k}{\partial x}$ may be written as follows:

$$\begin{aligned}\frac{\partial \rho_k}{\partial x} &= \frac{W_k}{\mathcal{R}T}\frac{\partial p}{\partial x} - \frac{W_k p}{\mathcal{R}T^2}\frac{\partial T}{\partial x}\\ &= \frac{\rho_k}{p}\frac{\partial p}{\partial x} - \frac{\rho_k}{T}\frac{\partial T}{\partial x}\end{aligned}\tag{25}$$

Therefore Equation 20 may be evaluated to be:

$$\begin{aligned}\frac{\partial}{\partial x}(h_1 - h_2) &= \Big[\Big(\frac{c_1^2}{Y_1} + \frac{c_2^2}{Y_2}\Big) - \Big(\frac{W_1 c_1^2}{Y_1} + \frac{W_2 c_2^2}{Y_2}\Big) + \frac{(c_1^2 - c_2^2)(\rho_1 - \rho_2)W^2}{\rho W_1 W_2}\Big]\frac{\partial Y_1}{\partial x} + \frac{(c_1^2 - c_2^2)}{p}\frac{\partial p}{\partial x} - \frac{(c_1^2 - c_2^2)}{T}\frac{\partial T}{\partial x}\\ &= \Big[\frac{Y_2(1 - W_1)c_1^2 + Y_1(1 - W_2)c_2^2}{Y_1 Y_2} + \frac{(c_1^2 - c_2^2)(\rho_1 - \rho_2)W^2}{\rho W_1 W_2}\Big]\frac{\partial Y_1}{\partial x} + \frac{(c_1^2 - c_2^2)}{p}\frac{\partial p}{\partial x} - \frac{(c_1^2 - c_2^2)}{T}\frac{\partial T}{\partial x}\\ &= E_{Y_1 Y_1}\frac{\partial Y_1}{\partial x} + E_{Y_1 T}\frac{\partial T}{\partial x} + E_{Y_1 p}\frac{\partial p}{\partial x}\end{aligned}\tag{26}$$

This allows for the terms $E_{Y_1Y_1}$, E_{Y_1T} and E_{Y_1p} to be determined, which means that the coefficients χ_{ij} can be evaluated through use of Equation 18. Noting that $E_{Y_1} = \mu$ and $E_s = T$, the thermal flux is:

$$\begin{aligned} q &= E_{Y_1}E_{\tilde{w}} + E_sE_J \\ &= \mu E_{\tilde{w}} + TE_J \\ &= -\mu\chi_{11}\frac{\partial \mu}{\partial x} - \mu\chi_{12}\frac{\partial T}{\partial x} - T\chi_{21}\frac{\partial \mu}{\partial x} - T\chi_{22}\frac{\partial T}{\partial x} \end{aligned} \tag{27}$$

Also, given that $E_{\tilde{w}} = \mathcal{J}$ then q can be written as:

$$q = \Big(\mu + \frac{\chi_{21}}{\chi_{11}}T\Big)\mathcal{J} - \frac{\chi_{11}\chi_{22} - \chi_{12}\chi_{21}}{\chi_{11}}T\frac{\partial T}{\partial x} \tag{28}$$

Which means that the thermal conductivity coefficient κ is equal to:

$$\kappa = \frac{\chi_{11}\chi_{22} - \chi_{12}\chi_{21}}{\chi_{11}}T \tag{29}$$

Given that the mass flux $\mathcal{J}$ takes the form:

$$\begin{aligned} \mathcal{J} &= -\chi_{11}\mu_{Y_1}\frac{\partial Y_1}{\partial x} - (\chi_{12} - \chi_{11}\mu_T)\frac{\partial T}{\partial x} - \chi_{11}\mu_p\frac{\partial p}{\partial x} \\ &= -\rho D\Big(\frac{\partial Y_1}{\partial x} + \frac{k_T}{T}\frac{\partial T}{\partial x} + \frac{k_p}{p}\frac{\partial p}{\partial x}\Big) \end{aligned} \tag{30}$$

Then χ_{11}, $\chi_{12} = \chi_{21}$ and χ_{22} can be found as follows:

$$\begin{aligned} \chi_{11} &= \frac{\rho D}{\mu_{Y_1}} \\ \chi_{12} &= \Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)\chi_{11} \\ \chi_{22} &= \frac{\kappa}{T} + \frac{\chi_{12}\chi_{21}}{\chi_{11}} \end{aligned} \tag{31}$$

where $\mu_{Y_1} = E_{Y_1Y_1}$, $\mu_T = E_{Y_1T}$ and $\mu_p = E_{Y_1p}$ are found using Equation 26. Thus the kinetic coefficients θ_{ij} are given by:

$$\begin{aligned} \begin{bmatrix} \theta_{11} & \theta_{12} \\ \theta_{21} & \theta_{22} \end{bmatrix} &= \begin{bmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \frac{\rho D}{\mu_{Y_1}} & \Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)\frac{\rho D}{\mu_{Y_1}} \\ \Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)\frac{\rho D}{\mu_{Y_1}} & \frac{\kappa}{T} + \Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)^2\frac{\rho D}{\mu_{Y_1}} \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \frac{\mu_{Y_1}}{\rho D} + \Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)^2\frac{T}{\kappa} & -\Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)\frac{T}{\kappa} \\ -\Big(\frac{k_T}{T}\mu_{Y_1} - \mu_T\Big)\frac{T}{\kappa} & \frac{T}{\kappa} \end{bmatrix} \end{aligned} \tag{32}$$

This completes the analysis of the stiff relaxation limit. The generating system can now be used to formulate governing equations in terms of the state parameters, as all thermodynamic forces have been expressed in terms of derivatives of the total energy E, and all of the model kinetic coefficients have been defined.

4 Governing equations in terms of parameters of state

For implementation in a numerical method it is more convenient to write the governing equations in terms of the parameters of state defined in Section 2. Prior to this, a hyperbolic formulation of viscosity will be added to the model by deriving a one-dimensional form of the evolution equations for the distortion tensor in [10, 11]. These equations can be added to this existing equation set without affecting any of the previous derivations, thus providing a complete hyperbolic description of a viscous binary mixture in one dimension which will be written in terms of the state parameters for numerical implementation.

4.1 One-dimensional equations for distortion

One-dimensional equations for the distortion tensor $\boldsymbol{A}$ can be derived from the three-dimensional equations presented in [11] and read as:

$$\begin{aligned}\frac{\partial A_{11}}{\partial t}+\frac{\partial u A_{11}}{\partial x}&=-\frac{\Psi_{11}}{\phi}\\ \frac{\partial A_{22}}{\partial t}+u\frac{\partial A_{22}}{\partial x}&=-\frac{\Psi_{22}}{\phi}\\ \frac{\partial A_{33}}{\partial t}+u\frac{\partial A_{33}}{\partial x}&=-\frac{\Psi_{33}}{\phi}\end{aligned} \tag{33}$$

where $\Psi_{ik}=E_{A_{ik}}$ and ϕ is some function of the strain dissipation time τ. These equations are obtained under the assumption that the fluid flows with velocity u only in the x-direction and hence $A_{ij}=0$, $i\neq j$. Assuming that $A_{22}=A_{33}$ due to isotropy, and denoting $A_1=A_{11}$, $A_2=A_{22}$ gives:

$$\begin{aligned}\frac{\partial A_{1}}{\partial t}+\frac{\partial u A_{1}}{\partial x}&=-\frac{\Psi_{11}}{\phi}\\ \frac{\partial A_{2}}{\partial t}+u\frac{\partial A_{2}}{\partial x}&=-\frac{\Psi_{22}}{\phi}\end{aligned} \tag{34}$$

As per [11], the relaxation terms on the right-hand side are given in matrix form as:

$$\boldsymbol{\Psi}=\frac{\partial E}{\partial \boldsymbol{A}}=c_s^2\boldsymbol{A}\mathrm{dev}(\boldsymbol{G}),\quad G=\boldsymbol{A}\boldsymbol{A}^T \tag{35}$$

where c_s is the shear sound velocity, that is, the characteristic velocity of propagation of transverse perturbations. Since $A_{ij}=0$, $i\neq j$ then $\boldsymbol{G}$ is given by:

$$\boldsymbol{G}=\begin{bmatrix}A_1^2 & 0 & 0\\ 0 & A_2^2 & 0\\ 0 & 0 & A_3^2\end{bmatrix} \tag{36}$$

and the deviatoric part of $\boldsymbol{G}$ is given by:

$$\mathrm{dev}(\boldsymbol{G})=\boldsymbol{G}-\frac{1}{3}\mathrm{Tr}(\boldsymbol{G})=\begin{bmatrix}\frac{2}{3}(A_1^2-A_2^2) & 0 & 0\\ 0 & -\frac{1}{3}(A_1^2-A_2^2) & 0\\ 0 & 0 & -\frac{1}{3}(A_1^2-A_2^2)\end{bmatrix} \tag{37}$$

Therefore the energy gradients are:

$$\begin{aligned}\Psi_{11}&=c_s^2A_1\frac{2}{3}(A_1^2-A_2^2)\\ \Psi_{22}&=-c_s^2A_2\frac{1}{3}(A_1^2-A_2^2)\end{aligned} \tag{38}$$

The strain relaxation source term ϕ is defined following [11]:

$$\phi=\tau\frac{c_s^2}{3}\det(\boldsymbol{A})^{\frac{5}{3}}=\tau\frac{c_s^2}{3}(A_1A_2^2)^{\frac{5}{3}} \tag{39}$$

4.2 Modification of the momentum equation

The inclusion of equations for the distortion tensor also requires that a shear stress tensor is added to the momentum equations. Since the fluid is assumed to flow only in the x-direction, there is only one momentum equation:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial(\rho u^2 + p - \sigma_{11})}{\partial x} = 0 \tag{40}$$

Following [11], the shear stress tensor $\boldsymbol{\sigma}$ is computed as:

$$\boldsymbol{\sigma} = -\rho \boldsymbol{A}^T \frac{\partial E}{\partial \boldsymbol{A}} = -\rho c_s^2 \boldsymbol{G} \mathrm{dev}(\boldsymbol{G}) \tag{41}$$

Thus, in matrix form $\boldsymbol{\sigma}$ is given by:

$$\boldsymbol{\sigma} = \begin{bmatrix} -\rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2) & 0 & 0 \\ 0 & \rho c_s^2 A_2^2 \frac{1}{3}(A_1^2 - A_2^2) & 0 \\ 0 & 0 & \rho c_s^2 A_2^2 \frac{1}{3}(A_1^2 - A_2^2) \end{bmatrix} \tag{42}$$

and therefore:

$$\sigma_{11} = -\rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2) \tag{43}$$

4.3 Complete system of equations

The full set of state parameters describing the mixture in one spatial dimension is now:

$$\{\rho, Y_1, u, A_1, A_2, \tilde{w}, J, s\}$$

The total energy is defined as per Equation 10, with the definition of the non-equilibrium energy extended to include the components of the distortion tensor:

$$\begin{aligned} E_2(A_1, A_2, \tilde{w}, J) &= \frac{c_s^2}{4} G_{ij}^{\mathrm{TF}} G_{ij}^{\mathrm{TF}} + \frac{\alpha^2}{2} J^2 + \frac{\beta^2}{2} \tilde{w}^2 \\ &= \frac{c_s^2}{6}(A_1^2 - A_2^2)^2 + \frac{\alpha^2}{2} J^2 + \frac{\beta^2}{2} \tilde{w}^2 \end{aligned} \tag{44}$$

where $G_{ij}^{\mathrm{TF}} = \mathrm{dev}(\boldsymbol{G})$ is the trace-free part of $\boldsymbol{G}$. The parameter c_s cannot be determined explicitly, but via a formal asymptotic expansion of the tensor $\boldsymbol{G}$ in terms of the small parameter τ, it can be shown that (to first order in τ) the conventional dynamic viscosity coefficient $\eta = C_0 \tau c_s^2$, where C_0 is some additional constant. In order to recover both parameters, experimental measurements of high frequency sound propagation are required (see [11] for further details). Similarly, the parameters α and β are not known explicitly, but the products $\epsilon\alpha^2$ and $\epsilon\beta^2$ can be connected to the conventional transport coefficients for thermal and mass diffusion, where ϵ is some small relaxation parameter (each process will have a characteristic relaxation time but these cannot be defined explicitly due to coupling as noted in Section 3). This is not trivial to do and will be the subject of further work.

Therefore the complete set of equations in one dimension, including the effects of viscosity, diffusion and conductivity, is given as follows:

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0\\
&\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x}\Big(\rho Y_1 u + \beta^2 \tilde{w}\Big) = 0\\
&\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}\Big(\rho u^2 + p + \rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2)\Big) = 0\\
&\frac{\partial A_1}{\partial t} + \frac{\partial u A_1}{\partial x} = -\frac{2(A_1^2 - A_2^2)}{\tau (A_1 A_2^5)^{\frac{2}{3}}}\\
&\frac{\partial A_2}{\partial t} + u\frac{\partial A_2}{\partial x} = -\frac{A_2(A_1^2 - A_2^2)}{\tau (A_1^5 A_2^7)^{\frac{1}{3}}}\\
&\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x}\Big(\rho \tilde{w} u + h_1 - h_2\Big) = -\theta_{11}\beta^2 \tilde{w} - \theta_{12}\alpha^2 J\\
&\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x}\Big(\rho J u + T\Big) = -\theta_{21}\beta^2 \tilde{w} - \theta_{22}\alpha^2 J\\
&\frac{\partial \rho s}{\partial t} + \frac{\partial}{\partial x}\Big(\rho s u + \alpha^2 J\Big) = Q
\end{aligned}
\tag{45}
$$

where now the entropy production Q is given by:

$$
Q = \frac{1}{E_s}\Big(\frac{1}{\phi}(\psi_{11}^2 + \psi_{22}^2) + \theta_{11} E_{\tilde{w}}^2 + 2\theta_{12} E_{\tilde{w}} E_J + \theta_{22} E_J^2\Big) \geq 0 \tag{46}
$$

where θ_{ij} are given by Equation 32. For numerical implementation it is better to solve the following set of equations:

$$
\begin{aligned}
&\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x}\Big(\rho Y_1 u + \beta^2 \tilde{w}\Big) = 0\\
&\frac{\partial \rho Y_2}{\partial t} + \frac{\partial}{\partial x}\Big(\rho Y_2 u - \beta^2 \tilde{w}\Big) = 0\\
&\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}\Big(\rho u^2 + p + \rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2)\Big) = 0\\
&\frac{\partial A_1}{\partial t} + \frac{\partial u A_1}{\partial x} = -\frac{2(A_1^2 - A_2^2)}{\tau (A_1 A_2^5)^{\frac{2}{3}}}\\
&\frac{\partial A_2}{\partial t} + u\frac{\partial A_2}{\partial x} = -\frac{A_2(A_1^2 - A_2^2)}{\tau (A_1^5 A_2^7)^{\frac{1}{3}}}\\
&\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x}\Big(\rho \tilde{w} u + h_1 - h_2\Big) = -\theta_{11}\beta^2 \tilde{w} - \theta_{12}\alpha^2 J\\
&\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x}\Big(\rho J u + T\Big) = -\theta_{21}\beta^2 \tilde{w} - \theta_{22}\alpha^2 J\\
&\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x}\Big(\rho E u + \big(p + \rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2)\big)u + \beta^2 (h_1 - h_2)\tilde{w} + \alpha^2 T J\Big) = 0
\end{aligned}
\tag{47}
$$

This system of equations cannot be written in a fully conservative form when the equations for the distortion tensor are included, however recent advances in path-conservative methods for non-conservative systems provide a suitable approach for discretisation [21]. Indeed, when considering multispecies (or more generally multiphase) systems it is necessary to discretise the colour function in a non-conservative manner in order to preserve pressure equilibrium across an isolated contact surface [22], hence the fact that the distortion tensor equations are non-conservative is less of a hindrance to numerical implementation than may first appear. Another difficult aspect of this system when considering an appropriate numerical method to use is the stiffness of the source terms. One option is to use Strang time splitting [23], which allows a stiff ODE integrator to be used for the source terms, however a more efficient and promising approach is the family of high order one-step ADER schemes (see [24, 25, 26, 27] and references within). Future work will address the application of these methods to the current system of equations.

5 Conclusion and future work

A reformulation of the compressible multicomponent Navier–Stokes equations has been presented in the framework of thermodynamically compatible conservation laws. The resulting equation set is a first-order hyperbolic system containing stiff source terms and has been presented in complete detail for one spatial dimension. Closure relations and expressions for the kinetic coefficients were also presented, along with the final set of governing equations in terms of the parameters of state.

This work forms a small part of a much greater goal; the formulation of a three-dimensional, hyperbolic, two-phase, two-pressure, two-velocity, two-temperature model for viscous, miscible and compressible fluids and its numerical implementation within a high-order, multidimensional finite volume framework. The next steps towards this goal will be the numerical implementation of the current set of equations, using the methods discussed in Section 4.3, and a comparison with the conventional governing equations using a rigorous set of one-dimensional test cases. Once this has been achieved, this model will be used to assist in determining the necessary parameters and coefficients of a more general single entropy model for two-phase flow (similar in form to that presented in [17]), which is a better candidate for extension to multiple dimensions and numerical implementation with very high order methods.

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