Analysis and Approximation of Multicomponent Gas Mixtures

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Abstract. We consider a generalized system of Euler equations that describes the inviscid flow of a mixture of different gases. Systems of conservation laws of this type occur typically in the context of the numerical simulation of reacting gas flows. Results concerning the mathematical properties of the above model are presented. It turns out that a simple property of the thermodynamical equation of state ensures the hyperbolicity of the equation. The theoretical investigations are complemented by a numerical simulation of the Richtmyer-Meshkov instability.

1 Introduction

This article is devoted to theoretical aspects as well as to the numerical solution of a generalized system of Euler equations in several space dimensions. The nonlinear system describes the nonstationary inviscid flow of a compressible mixture consisting of K different gases. It arises from the usual Euler equations by replacing the continuity equation for a single ideal gas by continuity equations for each component of the mixture. Furthermore, a general thermodynamical equation of state and a caloric equation of state for the representation of the pressure and of the specific enthalpy, respectively, close the system. These quantities usually depend on the K partial densities and on the temperature.

Interest in conservation laws of the described type is mainly motivated by its importance in the context of the numerical approximation of gas flows that are coupled with chemical reactions [3].

The model can also be used for the simulation of the deformation of a curved contact discontinuity between a light and a heavy gas that is accelerated by an incoming shock wave from the light gas side [6, 7, 8].

Furthermore, it is very interesting to understand the complex behaviour of generalizations for numerical schemes applied to gas mixtures [1, 2, 10].

2 The Mathematical Model

The mathematical model for the inviscid flow of a gas mixture made up of K different components is described by the differential form of a system of conservation laws consisting of $K+d+1$ equations. The first K equations represent the conservation of mass for each component, the remaining $d+1$ relations express the conservation of momentum and energy.

The incorporation of source terms for the description of chemical reactions by Arrhenius kinetics [11] will be considered in a forthcoming paper.

$$\frac{\partial \vec{\mathbf{U}}}{\partial t}(\vec{x},t) + \sum_{j=1}^{d} \frac{\partial \vec{\mathbf{F}}_j}{\partial x_j}(\vec{\mathbf{U}}(\vec{x},t)) = \vec{\mathbf{0}}$$

$$\vec{x} \in \Omega \subset \mathbb{R}^d, \;\; d = 1,2,3, \;\; t \geq 0$$

$$\vec{\mathbf{U}}(\vec{x},0) = \vec{\mathbf{U}}^o(\vec{x}) \;\; + \text{Boundary conditions}$$

The vector of conservative variables and the flux vectors are denoted by $\vec{\mathbf{U}}$ and $\vec{\mathbf{F}}_j$, respectively. For each component of the mixture there is a partial density ρ_k. The sum of the partial densities is just the total density ρ of the mixture. Additionally, we use the notations $\vec{v} = (v_1, \ldots, v_d)^{\mathrm{T}} \in \mathbb{R}^d$ for the velocity, E for the total energy, p for the pressure, T for the temperature, h for the specific enthalpy and H for the total enthalpy with

$$H = E + \frac{p}{\rho} \;\; .$$

Thus, $\vec{\mathbf{U}}$ and $\vec{\mathbf{F}}_j$ are defined in the following way.

$$\vec{\mathbf{U}}(\vec{x},t) = (\rho_1, \ldots, \rho_K, \rho\vec{v}^{\,\mathrm{T}}, \rho E)^{\,\mathrm{T}}$$

$$\vec{\mathbf{F}}_j(\vec{\mathbf{U}}) = \Big(v_j(\rho_1, \ldots, \rho_K)\,,\, \rho v_j \vec{v}^{\,\mathrm{T}} + p\vec{e}_j^{\,\mathrm{T}}\,,\, v_j(\rho E + p)\Big)^{\mathrm{T}}$$

In the above definition $\vec{e}_j$ denotes the j-th unity vector in $\mathbb{R}^d$. Naturally, the pressure as well as the partial densities have to be positive.

The pressure that occurs in the definition of the flux vectors, is not a conservative variable. Consequently, further relations are necessary to complete the conservation law. These relations are usually given as the thermodynamical equation of state and the caloric equation of state that describe the pressure and the specific enthalpy as functions of a complete set of thermodynamical quantities but not with respect to the conservative variables. There are various possibilities to choose the set of independent thermodynamical variables [5, 9]. We use the partial densities and the temperature.

$$p = p(\rho_1, \ldots, \rho_K, T) \qquad h = h(\rho_1, \ldots, \rho_K, T)$$

To compute the flux vectors and the Jacobian matrices and to check the properties of the conservation law a representation of the pressure as a function of conservative variables has to be possible. The following lemma can be proved without further assumptions for the form of the equations of state.

Lemma 1:

1. Suppose the inequality
$$\rho\,\frac{\partial h}{\partial T} - \frac{\partial p}{\partial T} \neq 0$$
is satisfied for all possible arguments, then temperature and pressure are uniquely defined by each admissible state vector $\vec{\mathbf{U}}$:
$$T = T(\vec{\mathbf{U}}) \;\;\Rightarrow\;\; p = \tilde{p}(\vec{\mathbf{U}}) \equiv p(\rho_1, \ldots, \rho_K, T(\vec{\mathbf{U}}))$$

2. For the partial derivatives of $\tilde{p}$ the following statements are true:
$$\frac{\partial \tilde{p}}{\partial(\rho v_j)} + v_j \frac{\partial \tilde{p}}{\partial(\rho E)} = 0 \qquad j = 1, \ldots, d \qquad \Box$$

For the proof of the lemma we use some fundamental relations from thermodynamics and the implicit function theorem. For the standard case of an ideal polytropic gas the condition for the first statement is fulfilled because in this case the left hand side of the inequality is equal to the product of the density and the specific heat at constant volume. Note, however, that the function $\tilde{p}$ is, in general, defined via an implicit relation.

For the description of the further results some auxiliary notations are required. Let $\mathbf{I}_K$ and $\mathbf{I}_d$ denote the unity matrices in $\mathbb{R}^{K,K}$ and $\mathbb{R}^{d,d}$, respectively. Using $Y_k := \rho_k/\rho$ for the designation of the mass fractions of the components of the mixture we define the following quantities.

$$\begin{array}{rcll}
\vec{0} & := & (0, \ldots, 0)^{\mathrm{T}} & \in \mathbb{R}^K \\
\vec{1} & := & (1, \ldots, 1)^{\mathrm{T}} & \in \mathbb{R}^K \\
\vec{Y} & := & (Y_1, \ldots, Y_K)^{\mathrm{T}} & \in \mathbb{R}^K \\
\vec{\tilde{p}}_\rho & := & \left(\frac{\partial \tilde{p}}{\partial \rho_1}, \ldots, \frac{\partial \tilde{p}}{\partial \rho_K}\right)^{\mathrm{T}} & \in \mathbb{R}^K \\
\tilde{p}_{\rho E} & := & \frac{\partial \tilde{p}}{\partial \rho E} & \in \mathbb{R}
\end{array}$$

The above conservation law is called hyperbolic, if the matrix
$$\mathbf{A}(\vec{\mathbf{U}}, \vec{\kappa}) := \sum_{j=1}^{d} \kappa_j \,\frac{\partial \vec{\mathbf{F}}_j}{\partial \vec{\mathbf{U}}} \in \mathbb{R}^{K+d+1,K+d+1}$$

has only real eigenvalues and a complete system of eigenvectors for all states $\vec{\mathbf{U}} \in \mathbb{R}^{K+d+1}$ and for any direction $\vec{\kappa} \in \mathbb{R}^d$. The Jacobian matrices of the flux vectors with respect to the conservative variables can be written in the general form

$$\frac{\partial \vec{\mathbf{F}}_j}{\partial \vec{\mathbf{U}}} = \begin{pmatrix} v_j \left(\mathbf{I}_K - \vec{Y} \cdot \vec{1}^{\,\mathsf{T}} \right) & \vec{Y} \cdot \vec{e}_j^{\,\mathsf{T}} & \vec{0} \\ \vec{e}_j \cdot \vec{\tilde{p}}_\rho^{\,\mathsf{T}} - v_j \;\; \vec{v} \cdot \vec{1}^{\,\mathsf{T}} & \vec{v} \cdot \vec{e}_j^{\,\mathsf{T}} - \tilde{p}_{\rho E} \;\; \vec{e}_j \cdot \vec{v}^{\,\mathsf{T}} + v_j \;\; \mathbf{I}_d & \tilde{p}_{\rho E} \;\; \vec{e}_j \\ v_j \left(\vec{\tilde{p}}_\rho - H \;\; \vec{1}^{\,\mathsf{T}} \right) & H \;\; \vec{e}_j^{\,\mathsf{T}} - v_j \;\; \tilde{p}_{\rho E} \, \vec{v}^{\,\mathsf{T}} & v_j \left(1 + \tilde{p}_{\rho E}\right) \end{pmatrix} .$$

For the calculation of these matrices no special form of the equations of state is needed. They only depend on the partial derivatives of the function $\tilde{p}$, that describes the pressure with respect to the conservative variables. Combining these results, one gets

$$\mathbf{A}(\vec{\mathbf{U}}, \vec{\kappa}) =$$

$$\begin{pmatrix} (\vec{v}, \vec{\kappa}) \left(\mathbf{I}_K - \vec{Y} \cdot \vec{1}^{\,\mathsf{T}} \right) & \vec{Y} \cdot \vec{\kappa}^{\,\mathsf{T}} & \vec{0} \\ \vec{\kappa} \cdot \vec{\tilde{p}}_\rho^{\,\mathsf{T}} - (\vec{v}, \vec{\kappa}) \;\; \vec{v} \cdot \vec{1}^{\,\mathsf{T}} & \vec{v} \cdot \vec{\kappa}^{\,\mathsf{T}} - \tilde{p}_{\rho E} \;\; \vec{\kappa} \cdot \vec{v}^{\,\mathsf{T}} + (\vec{v}, \vec{\kappa}) \;\; \mathbf{I}_d & \tilde{p}_{\rho E} \;\; \vec{\kappa} \\ (\vec{v}, \vec{\kappa}) \left(\vec{\tilde{p}}_\rho - H \;\; \vec{1}^{\,\mathsf{T}} \right) & H \;\; \vec{\kappa}^{\,\mathsf{T}} - (\vec{v}, \vec{\kappa}) \;\; \tilde{p}_{\rho E} \;\; \vec{v}^{\,\mathsf{T}} & (\vec{v}, \vec{\kappa}) \left(1 + \tilde{p}_{\rho E}\right) \end{pmatrix}$$

$$\text{with} \quad \vec{\kappa} = (\kappa_1, \ldots, \kappa_d)^{\,\mathsf{T}} \quad \text{and} \quad (\vec{v}, \vec{\kappa}) := \sum_{j=1}^{d} v_j \kappa_j \quad .$$

It turns out, that the properties of the matrix function $\mathbf{A}(\vec{\mathbf{U}}, \vec{\kappa})$ may be described in a purely algebraic way without supposing any concrete shape of the equations of state.

Lemma 2: If the inequality

$$a := \sum_{k=1}^{K} \frac{\rho_k}{\rho} \frac{\partial \tilde{p}}{\partial \rho_k} + \left(h - \frac{|\vec{v}|^2}{2} \right) \frac{\partial \tilde{p}}{\partial (\rho E)} > 0$$

is satisfied, the matrix $\mathbf{A}(\vec{\mathbf{U}}, \vec{\kappa})$ has only real eigenvalues and a complete system of eigenvectors, i.e. the conservation law is hyperbolic. □

The eigenvalues are

$$\begin{aligned} \lambda_1 = \ldots = \lambda_{K+d-1} &= (\vec{v}, \vec{\kappa}) \ , \\ \lambda_{K+d} &= (\vec{v}, \vec{\kappa}) + |\vec{\kappa}|\sqrt{a} \\ \text{and} \quad \lambda_{K+d+1} &= (\vec{v}, \vec{\kappa}) - |\vec{\kappa}|\sqrt{a} \ . \end{aligned}$$

One of the eigenvalues has a $K+d-1$ dimensional eigenspace, the others are simple eigenvalues. A detailed computation gives the corresponding eigenvectors and the matrix for the similarity transformation of $\mathbf{A}(\vec{\mathbf{U}}, \vec{\kappa})$ onto diagonal form.

The quantity a may also be described in dependence on the partial derivatives of the thermodynamical representation of the pressure and the specific enthalpy.

$$a = \frac{\frac{\partial h}{\partial T} \sum_{k=1}^{K} \rho_k \frac{\partial p}{\partial \rho_k} - \frac{\partial p}{\partial T} \sum_{k=1}^{K} \rho_k \frac{\partial h}{\partial \rho_k}}{\rho \frac{\partial h}{\partial \rho_k} - \frac{\partial p}{\partial \rho_k}}$$

We note, that in the case of an ideal polytropic gas a is simply the square of the local speed of sound.

Further investigations concern conclusions from the Rankine-Hugoniot relations for the considered model. We can proof that all mass fractions Y_k have to be continuous at discontinuities of shock type. Mass fractions can only jump across a contact discontinuity.

Moreover for $d = 1$ the multiple eigenvalue has exactly two Riemann invariants, velocity and pressure. The mass fractions are Riemann invariants of the two simple eigenvalues, i.e. the mass fractions are constant across a rarefaction wave. These statements are true for arbitrary equations of state. The form of the remaining Riemann invariants of the simple eigenvalues for a gas mixture depends on the representation of the specific heats of the components.

The following equations of state describe a mixture of K ideal gases.

$$p(\rho_1, \ldots, \rho_K, T) = \mathcal{R}T \sum_{k=1}^{K} \frac{\rho_k}{W_k} \qquad h(\rho_1, \ldots, \rho_K, T) = \sum_{k=1}^{K} \frac{\rho_k}{\rho} h_k(T)$$

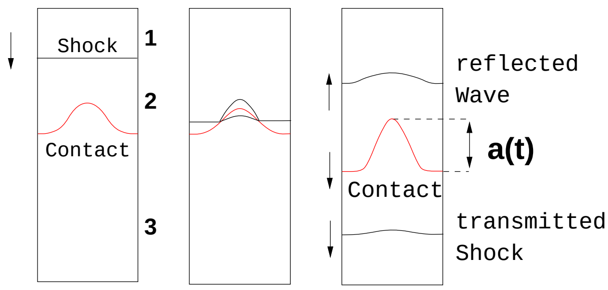
$$\text{with} \quad h_k(T) = \int_{T_o}^{T} c_{p,k}(\tau) d\tau + h_k^o$$

The molecular masses W_k, the specific heats at constant pressure $c_{p,k}(T)$ and the heats of formation h_k^o are given for all components. In addition, $\mathcal{R}$ denotes the universal gas constant.

3 Numerical Simulation

As an application results of a numerical simulation of the Richtmyer-Meshkov instability are presented. In an article from 1960 Richtmyer studied this problem by linearization techniques [8], ten years later Meshkov published first experimental observations. In the last few years further experimental as well as numerical results were published [6, 7].

The problem is to investigate the acceleration of a curved interface between a light and a heavy compressible gas mixture by an incoming plane shock wave. At the beginning, the interface has a sinusoidal shape. The heavy fluid protrudes into the light fluid. The shock comes from the light gas side and interacts with the contact discontinuity between the different media at rest. One wave is reflected, a shock is transmitted into the heavy gas and the contact discontinuity starts to move. Moreover, as time evolves the amplitude of the sinusoidal interface grows.



Interaction

We consider a mixture of Sulfur hexafluoride (SF_6) and air in two space dimensions ($K = d = 2$). For the molecular masses and the specific heats of SF_6 and air the following quantities are used:

$$\begin{aligned} W_{SF_6} &= 146.00 \, \frac{g}{mole}, & c_{p,SF_6} &= 689.70 \, \frac{Joule}{kg \cdot K} \\ W_{air} &= 29.08 \, \frac{g}{mole}, & c_{p,air} &= 1000.70 \, \frac{Joule}{kg \cdot K} \end{aligned}$$

The specific heats are supposed to be constant in this example. Furthermore, the heats of formation are set to zero for both components. It is important to note, that the specific heat of the mixture is not constant as in the standard Euler case. The same is true for the quotient of the specific heats for constant pressure and constant volume, usually denoted by γ.

At the starting point there are three different zones corresponding to the above figure. Within the first and the second domain the mixture consists of

95% air and 5% SF_6, within the remaining domain the opposite situation holds. Between the first and the second zone a pure shock wave is produced by the initial condition. Between the second and the third zone the initial condition describes a curved contact discontinuity at rest. The velocities at both sides of this line are zero. This discontinuity is an exact solution of the initial value problem.

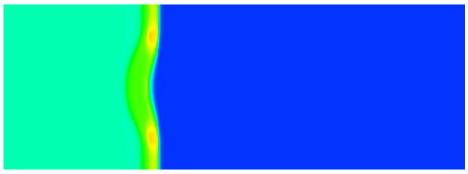
At the side walls of the channel reflection boundary conditions are used. At both ends of the tube an undisturbed outflow has to be guaranteed to prevent interactions of the moving curved contact line with shock waves that are generated by reflection at the end walls.

For the calculations a cell centered finite volume scheme on a quadrilateral mesh is applied. For the first order base method we constructed a generalized Steger-Warming scheme. It is supplemented by a bilinear recovery algorithm and a limiting procedure to achieve higher order.

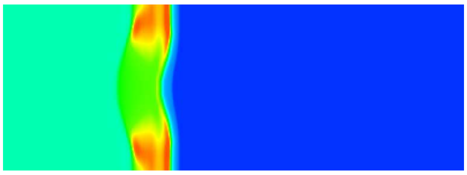
The implementation of the numerical method uses a flexible object-oriented software concept that allows a generic, grid- and dimension independent formulation of the algorithm via an abstract, iterator-based interface [4].

The expected effects are clearly demonstrated by a series of snap shots from the numerical simulation. The pictures show the partial density of air at several time layers. At dark zones ρ_{air} is low, within light areas it is high.

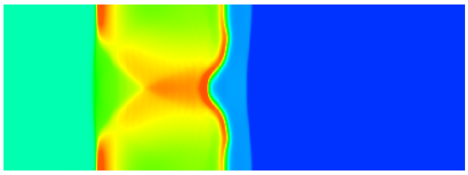
ρ_{air} at $t = 0.0$



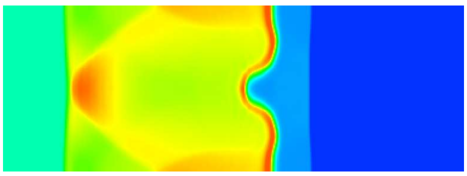
ρ_{air} at $t = 0.1146$



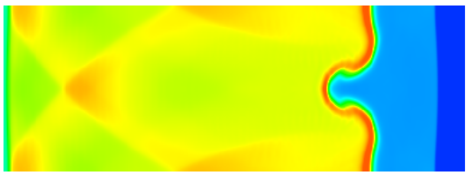
ρ_{air} at $t = 0.1746$



ρ_{air} at $t = 0.4026$



ρ_{air} at $t = 0.6006$



ρ_{air} at $t = 1.0032$

The mechanism for the development of the observed phenomena is roughly as follows. Immediately after the passage of the incoming shock the amplitude of the accelerated contact is somewhat less than at the beginning because of the overall compression of the fluid. In addition, over the first period the amplitude seems to be constant. As time goes on the generation of local pressure extrema causes a growing of the amplitude. The reflected shock is slightly diverging at the center of the sinusoidal perturbation whereas the transmitted shock wave is converging at the opposite side of the interface between the two fluids. This leads to a slight pressure deficiency in the lighter gas mixture and at the same time to a pressure excess in the heavy gas. At the sides of the sinusoidal interface the reverse situation holds.

During the further development we observe a complicated system of re-accelerations of the material interface by a cascade of secondary shocks generated by self-interactions at the reflected and the transmitted wave edges. These shocks periodically collide near the light gas side of the center of the curved contact line producing a higher pressure at this place and a reduction of the growth rate of the amplitude.

There are many interesting but, yet, open questions in the context of the Richtmyer-Meshkov instability concerning analytical as well as numerical problems.

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