Numerical simulation of the passive gas mixture flow

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Abstract. We work with the system of equations describing non-stationary compressible turbulent multicomponent flow in the gravitational field, and we focus on the numerical solution of these equations. In these computations we assume the mixture of perfect inert gases. The thermodynamic constants are functions in time and space. The finite volume method is used. In order to solve the local boundary problem at each mesh face, we use the original analysis of the exact solution of the Riemann problem. The roughness of the surface is simulated via the specific dissipation at the wall. We show the computational results obtained with the own-developed code (C,FORTRAN) for the solution of the 3D compressible turbulent mixture flow. The originality of this work lies with the special handling of the boundary conditions, which shows superior behavior, and own computational code.

1 Introduction

The aim of this work is to numerically simulate complicated behaviour of the perfect gas mixture. In this contribution we consider the Reynolds- Averaged Navier-Stokes equations with the $k-\omega$ model of turbulence. This system is equipped with the equation of state in more general form, and with the mass conservation of the additional gas specie.

2 Formulation of the Equations

We consider the conservation laws for viscous compressible turbulent flow of ideal gas with the zero heat sources in a domain $\Omega \in \mathbb{R}^N$, and time interval $(0, T)$, with $T > 0$. The system of the Reynolds-Averaged Navier-Stokes equations in 3D has the form

$$\frac{\partial \mathbf{w}}{\partial t} + \sum_{s=1}^3 \frac{\partial \mathbf{f}_s(\mathbf{w})}{\partial x_s} = \sum_{s=1}^3 \frac{\partial \mathbf{R}_s(\mathbf{w}, \nabla \mathbf{w})}{\partial x_s} + \mathbf{S} \quad \text{in } Q_T = \Omega \times (0, T). \quad (1)$$

Here x_1, x_2, x_3 are the space coordinates, t the time, $\mathbf{w} = \mathbf{w}(x, t) = (\varrho, \varrho v_1, \varrho v_2, \varrho v_3, E)^T$ is the state vector, $\mathbf{f}_s = (\varrho v_s, \varrho v_s v_1 + \delta_{s1} p, \varrho v_s v_2 + \delta_{s2} p, \varrho v_s v_3 + \delta_{s3} p, (E + p) v_s)^T$ are the inviscid fluxes, $\mathbf{R}_s = (0, \tau_{s1}, \tau_{s2}, \tau_{s3}, \sum_{r=1}^3 \tau_{sr} v_r + C_k \partial \theta / \partial x_s)^T$ are the viscous fluxes, $\mathbf{S}$ are additional sources. $\mathbf{v} = (v_1, v_2, v_3)^T$ denotes the velocity vector, ϱ is the density, p the pressure, θ the absolute temperature, $E = \varrho e + \frac{1}{2} \varrho v^2$

the total energy. Further $\tau_{ij} = \begin{cases} (\mu + \mu_T) S_{ij}, & i \neq j \\ (\mu + \mu_T) S_{ij} - \frac{2}{3} \varrho k, & i = j \end{cases}$,

with $S_{11} = \frac{2}{3} (2 \frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3})$, $S_{12} = \frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}$, $S_{13} = \frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1}$, $S_{21} = S_{12}$, $S_{22} = \frac{2}{3} (-\frac{\partial v_1}{\partial x_1} + 2 \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3})$, $S_{23} = \frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2}$, $S_{31} = S_{13}$, $S_{32} = S_{23}$, $S_{33} = \frac{2}{3} (-\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} + 2 \frac{\partial v_3}{\partial x_3})$, where μ is the dynamic viscosity coefficient dependent on temperature, μ_T is the eddy-viscosity coefficient. For the specific

internal energy $e = c_v \theta$ we assume the caloric equation of state $e = p / (\varrho(\gamma - 1))$, c_v is the specific heat at constant volume, $\gamma > 1$ is called the *Poisson adiabatic constant*. The constant C_k denotes the heat conduction coefficient $C_k = (\frac{\mu}{P_r} + \frac{\mu_T}{P_{rT}}) c_v \gamma$, and P_r is laminar and P_{rT} is turbulent Prandtl constant number. In our application of flow in the gravitational field we set the source terms to $\mathbf{S} = (0, \varrho g_1, \varrho g_2, \varrho g_3, \varrho \mathbf{g} \cdot \mathbf{v})$, where $\mathbf{g} = (g_1, g_2, g_3)$ is the gravity vector. For the gas mixture with two species we use the Dalton's law for the total mixture pressure

$$p = p_1 + p_2,$$

where p_1 and p_2 are the partial pressures of the first and second component gas. Let ϱ_1 and ϱ_2 be the mass density of these components. Then the total mass density of mixture is

$$\varrho = \varrho_1 + \varrho_2.$$

Temperature θ is same for all gases in the mixture, and the equation of state holds

$$p_i = \varrho_i R_i \theta, \quad R_i = \frac{R_g}{m_i},$$

where $R_g = 8.3144621$ is universal gas constant, and m_i denotes the molar mass of the i th specie. We can introduce the species mass fractions Y_1, Y_2 , with $Y_1 = \frac{\varrho_1}{\varrho}$, $Y_2 = \frac{\varrho_2}{\varrho}$, it is $Y_1 + Y_2 = 1$. The thermodynamic constants of the mixture satisfy (using the decomposition of the internal specific energy and enthalpy)

$$\varrho c_p = \sum \varrho_i c_{pi}, \quad \varrho c_v = \sum \varrho_i c_{vi},$$

then the adiabatic constant γ , needed in the solution of (1), can be written as

$$\gamma = \frac{c_p}{c_v} = \frac{\sum Y_i c_{pi}}{\sum Y_i c_{vi}}.$$

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The system (1) is then extended with the conservation law of the mass for one gas component (specie)

$$\frac{\partial \varrho Y_1}{\partial t} + \frac{\partial \varrho Y_1 v_1}{\partial x_1} + \frac{\partial \varrho Y_1 v_2}{\partial x_2} + \frac{\partial \varrho Y_1 v_3}{\partial x_3} = \frac{\partial}{\partial x_1} \left(\sigma_C \mu_T \frac{\partial Y_1}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\sigma_C \mu_T \frac{\partial Y_1}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(\sigma_C \mu_T \frac{\partial Y_1}{\partial x_3} \right) \quad (2)$$

Here σ_C is diffusion coefficient. The mass conservation for the second specie is automatically satisfied via the system (1).

Here we assume the system (1),(2) equipped with the two-equation turbulent model $k-\omega$ (Kok), described in [1]. The effective turbulent viscosity is $\mu_T = \varrho k / \omega$.

$$\begin{aligned} \frac{\partial \varrho k}{\partial t} + \frac{\partial \varrho k v_1}{\partial x_1} + \frac{\partial \varrho k v_2}{\partial x_2} + \frac{\partial \varrho k v_3}{\partial x_3} &= P_k - \beta^* \varrho \omega k + \\ &+ \frac{\partial}{\partial x_1} \left((\mu + \sigma_k \mu_T) \frac{\partial k}{\partial x_1} \right) + \\ &+ \frac{\partial}{\partial x_2} \left((\mu + \sigma_k \mu_T) \frac{\partial k}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left((\mu + \sigma_k \mu_T) \frac{\partial k}{\partial x_3} \right), \quad (3) \end{aligned}$$

$$\begin{aligned} \frac{\partial \varrho \omega}{\partial t} + \frac{\partial \varrho \omega v_1}{\partial x_1} + \frac{\partial \varrho \omega v_2}{\partial x_2} + \frac{\partial \varrho \omega v_3}{\partial x_3} &= P_\omega - \beta \varrho \omega \omega + \\ &+ C_D + \frac{\partial}{\partial x_1} \left((\mu + \sigma_\omega \mu_T) \frac{\partial \omega}{\partial x_1} \right) + \\ &+ \frac{\partial}{\partial x_2} \left((\mu + \sigma_\omega \mu_T) \frac{\partial \omega}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left((\mu + \sigma_\omega \mu_T) \frac{\partial \omega}{\partial x_3} \right), \quad (4) \end{aligned}$$

where k the turbulent kinetic energy and ω the turbulent dissipation are functions of time t and space coordinates x_1, x_2, x_3 . The production terms P_k and P_ω are given by formulas

$$\begin{aligned} P_k &= \tau_{11} \frac{\partial v_1}{\partial x_1} + \tau_{12} \frac{\partial v_1}{\partial x_2} + \tau_{21} \frac{\partial v_2}{\partial x_1} + \tau_{22} \frac{\partial v_2}{\partial x_2} + \tau_{13} \frac{\partial v_1}{\partial x_3} + \\ &+ \tau_{31} \frac{\partial v_3}{\partial x_1} + \tau_{23} \frac{\partial v_2}{\partial x_3} + \tau_{32} \frac{\partial v_3}{\partial x_2} + \tau_{33} \frac{\partial v_3}{\partial x_3}, \\ P_\omega &= \frac{\alpha_\omega \omega P_k}{k}, \end{aligned}$$

where functions τ are defined in (1) with $\mu = 0$, $\alpha_\omega = \frac{\beta}{\beta^*} - \frac{\sigma_\omega \kappa^2}{\sqrt{\beta^*}}$ and $\sigma_k = \frac{2}{3}$, $\beta^* = 0.09$, $\beta = \frac{5}{6} \beta^*$, $\sigma_\omega = 0.5$, $\kappa = 0.41$. The cross-diffusion term C_D is defined as

$$C_D = \sigma_d \frac{\varrho}{\omega} \max \left\{ \frac{\partial k}{\partial x_1} \frac{\partial \omega}{\partial x_1} + \frac{\partial k}{\partial x_2} \frac{\partial \omega}{\partial x_2} + \frac{\partial k}{\partial x_3} \frac{\partial \omega}{\partial x_3}, 0 \right\},$$

where $\sigma_d = 0.5$ is constant.

3 Numerical Method

For the discretization of the system we proceed as described in [6]. We use either explicit or implicit finite volume method to solve the systems sequentially. Here we present the discretization of the system (1). By $\mathcal{Q}_h$ let us denote the polyhedral approximation of Ω . The system of the closed polyhedrons with mutually disjoint interiors $\mathcal{D}_h = \{D_i\}_{i \in J}$, where $J \subset \mathbb{Z}^+ = \{0, 1, \dots\}$ is an index set and $h > 0$, will

be called a *finite volume mesh*. This system $\mathcal{D}_h$ approximates the domain Ω , we write $\overline{\Omega}_h = \bigcup_{i \in J} D_i$. The elements $D_i \in \mathcal{D}_h$ are called the *finite volumes*. For two neighboring elements D_i, D_j we set $\Gamma_{ij} = \partial D_i \cap \partial D_j = \Gamma_{ji}$. Similarly, using the negative index j we may denote the boundary faces. Here we will work with the so-called *regular meshes*, i.e. the intersection of two arbitrary (different) elements is either empty or it consists of a common vertex or a common edge or a common face (in 3D). The boundary ∂D_i of each element D_i is

$$\partial D_i = \bigcup_{\Gamma_{ij} \in \Gamma_{D_i}} \Gamma_{ij}. \quad (5)$$

Here the set $\Gamma_{D_i} = \{\Gamma_{ij}; \Gamma_{ij} \subset \partial D_i\}$ forms the boundary ∂D_i . By $\mathbf{n}_{ij}$ let us denote the unit outer normal to ∂D_i on Γ_{ij} . Let us construct a partition $0 = t_0 < t_1 < \dots$ of the time interval $[0, T]$ and denote the time steps $\tau_k = t_{k+1} - t_k$. We integrate the system (1) over the set $D_i \times (t_k, t_{k+1})$. With the integral form of the equations we can study a flow with discontinuities, such as shock waves, too.

$$\begin{aligned} \int_{D_i} \int_{t_k}^{t_{k+1}} \frac{\partial \mathbf{w}}{\partial t} dx dt + \int_{t_k}^{t_{k+1}} \int_{D_i} \sum_{s=1}^3 \frac{\partial f_s(\mathbf{w})}{\partial x_s} dx dt &= \\ &= \int_{t_k}^{t_{k+1}} \int_{D_i} \sum_{s=1}^3 \frac{\partial R_s(\mathbf{w}, \nabla \mathbf{w})}{\partial x_s} dx dt \quad (6) \end{aligned}$$

Using the Green's theorem on D_i it is

$$\begin{aligned} \int_{D_i} \sum_{s=1}^3 \frac{\partial f_s(\mathbf{w})}{\partial x_s} dx &= \int_{\partial D_i} \sum_{s=1}^3 f_s(\mathbf{w}) n_s dS, \quad (7) \\ \int_{D_i} \sum_{s=1}^3 \frac{\partial R_s(\mathbf{w}, \nabla \mathbf{w})}{\partial x_s} dx &= \int_{\partial D_i} \sum_{s=1}^3 R_s(\mathbf{w}, \nabla \mathbf{w}) n_s dS. \end{aligned}$$

Here $\mathbf{n} = (n_1, n_2, n_3)$ is the unit outer normal to ∂D_i . Further we use (5), and we rewrite (6)

$$\begin{aligned} \int_{D_i} (\mathbf{w}(x, t_{k+1}) - \mathbf{w}(x, t_k)) dx + \\ \int_{t_k}^{t_{k+1}} \sum_{\Gamma_{ij} \in \Gamma_{D_i}} \int_{\Gamma_{ij}} \sum_{s=1}^3 (f_s(\mathbf{w}) - R_s(\mathbf{w}, \nabla \mathbf{w})) (n_{ij})_s dS dt &= 0 \quad (8) \end{aligned}$$

We define a finite volume approximate solution of the system studied (1) as a piecewise constant vector-valued functions $\mathbf{w}_h^k$, $k = 0, 1, \dots$, where $\mathbf{w}_h^k$ is constant on each element D_i , and t_k is the time instant. By $\mathbf{w}_i^k$ we denote the value of the approximate solution on D_i at time t_k . We approximate the integral over the element D_i

$$\int_{D_i} \mathbf{w}(x, t_k) dx \approx |D_i| \mathbf{w}_i^k. \quad (9)$$

Further we proceed with the approximation of the fluxes. Usually the flux $\sum_{s=1}^3 f_s(\mathbf{w})(n_{ij})_s |_{\Gamma_{ij}}$ is being approximated by a *numerical flux* at suitable time instant t_l

$$\sum_{s=1}^3 f_s(\mathbf{w})(n_{ij})_s |_{\Gamma_{ij}} \approx \mathbf{H}(\mathbf{w}_i^l, \mathbf{w}_j^l, \mathbf{n}_{ij}),$$

with $\mathbf{w}_i^l, \mathbf{w}_j^l$ denoting the approximate solution on the elements adjacent to the edge Γ_{ij} at the time instant t_l . In the case of a boundary face the vector $\mathbf{w}_j^l$ has to be specified.

Here we show the numerical flux based on the solution of the Riemann problem for the split Euler equations. By $w_{\Gamma_{ij}}^l$ let us denote the state vector w at the center of the edge Γ_{ij} at the time instant t_l , and let us suppose $w_{\Gamma_{ij}}^l$ is known. Evaluation of these values will be a question of the further analysis, here we use them to approximate the integrals with the one-point rule

$$\int_{\Gamma_{ij}} \sum_{s=1}^3 f_s(w(x, t_l))(n_{ij})_s dS \approx |\Gamma_{ij}| \sum_{s=1}^3 f_s(w_{\Gamma_{ij}}^l)(n_{ij})_s. \quad (10)$$

$$\int_{\Gamma_{ij}} \sum_{s=1}^3 R_s(w(x, t_l), \nabla w(x, t_l))(n_{ij})_s dS \approx |\Gamma_{ij}| \sum_{s=1}^3 R_s(w_{\Gamma_{ij}}^l, \nabla w_{\Gamma_{ij}}^l)(n_{ij})_s.$$

Here $\nabla w_{\Gamma_{ij}}^l$ denotes the ∇w at the center of the edge Γ_{ij} at time instant t_l . Now it is possible to approximate the system (8) by the following explicit finite volume scheme

$$\frac{|D_i|}{\tau_k} (w_i^{k+1} - w_i^k) + \sum_{\Gamma_{ij} \in \mathcal{F}_{D_i}} |\Gamma_{ij}| \sum_{s=1}^3 (f_s(w_{\Gamma_{ij}}^k) n_s - R_s(w_{\Gamma_{ij}}^k, \nabla w_{\Gamma_{ij}}^k) n_s) = 0 \quad (11)$$

With this finite volume formula one computes the values of the approximate solution at the time instant t_{k+1} , using the values from the time instant t_k , and by evaluating the values $w_{\Gamma_{ij}}^k$ at the faces Γ_{ij} . In order to achieve the stability of the used method, the time step τ_k must be restricted by the so-called CFL condition, see [4]. The crucial problem of this discretization lies with the evaluation of the edge values $w_{\Gamma_{ij}}^k$. Or one deals with the problem of finding the face fluxes $H(w_i^k, w_j^k, n_{ij})$. It is also possible to use the **implicit scheme**

$$\frac{|D_i|}{\tau_k} (w_i^{k+1} - w_i^k) + \sum_{\Gamma_{ij} \in \mathcal{F}_{D_i}} |\Gamma_{ij}| \left(H(w_i^{k+1}, w_j^{k+1}, n_{ij}) - \sum_{s=1}^3 R_s(w_{\Gamma_{ij}}^{k+1}, \nabla w_{\Gamma_{ij}}^{k+1}) n_s \right) = 0 \quad (12)$$

The crucial problem of this discretization lies with the evaluation of the face fluxes $H(w_i^{k+1}, w_j^{k+1}, n_{ij})$. One possibility is to use the linearization via the Taylor expansion of the vector function $H(wI, wJ, n)$, this was shown in [6]. One possibility of the face flux evaluation is to approximate the face values $w_{\Gamma_{ij}}^k$ and then compute the numerical flux

$$H_{ij}^k = \sum_{s=1}^3 f_s(w_{\Gamma_{ij}}^k)(n_{ij})_s. \quad (13)$$

To approximate the face values $w_{\Gamma_{ij}}^k$ at time instant t_k we solve the simplified system (14) in the vicinity of the face Γ_{ij} in time with the initial condition formed by the state vectors w_i^k and w_j^k . Using the rotational invariance of the Euler equations, the system is expressed in a new Cartesian coordinate system $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$ with the origin at the center of the gravity of Γ_{ij} and with the new axis $\tilde{x}_1$ in the direction of $n = (n_1, n_2, n_3)$, given by the face normal $n = n_{ij}$. Then the derivatives with respect to $\tilde{x}_2, \tilde{x}_3$ are neglected and we get the so-called split 3D Euler equations, see [4, page 138]:

$$\frac{\partial q}{\partial t} + \frac{\partial f_1(q)}{\partial \tilde{x}_1} = 0. \quad (14)$$

Fig. 1. Coordinate transformation for the inner edges in 2D.

The values w_i^k and w_j^k adjacent to the face Γ_{ij} are known, forming the initial conditions

$$q(\tilde{x}_1, 0) = q_L = \mathbb{Q} w_i^k, \quad \tilde{x}_1 < 0, \quad (15)$$

$$q(\tilde{x}_1, 0) = q_R = \mathbb{Q} w_j^k, \quad \tilde{x}_1 > 0. \quad (16)$$

The transformation matrix $\mathbb{Q}$ is defined in [6]. The problem (14), (15), (16) has a unique “solution” in $(-\infty, \infty) \times (0, \infty)$, the analysis can be found in [4, page 138]. Let $q_{RS}(q_L, q_R, \tilde{x}_1, t)$ denote the solution of this problem at the point $(\tilde{x}_1, t)$. We are interested in the solution of this local problem at the time axis, which is the sought solution in the local coordinates $q_{\Gamma_{ij}} = q_{RS}(q_L, q_R, 0, t)$. The backward transformation of the state vector $q_{\Gamma_{ij}}$ into the global coordinates is

$$w_{\Gamma_{ij}}^k = \mathbb{Q}^{-1} q_{\Gamma_{ij}} = \mathbb{Q}^{-1} q_{RS}(\mathbb{Q} w_i^k, \mathbb{Q} w_j^k, 0, t). \quad (17)$$

The constructed numerical flux can be written as

$$H(u, v, n) := \sum_{s=1}^3 f_s(\mathbb{Q}^{-1} q_{RS}(\mathbb{Q} u, \mathbb{Q} v, 0, t)) n_s. \quad (18)$$

Let Γ_{ij} be the face of the element D_i laying at the boundary of the computational area. To approximate the face values $w_{\Gamma_{ij}}^k$ at time instant t_k we solve the incomplete simplified system (14) in the vicinity of the face Γ_{ij} in time with the initial condition (15) determined by the state vector w_i^k . By adding properly chosen equations into the system (14), (15) it is possible to reconstruct the boundary state q_B such that the system (14), (15) has a unique solution at the boundary, see [3]. We will refer to these added equations as to **complementary conditions**. Several choices of the complementary conditions were discussed in [3], [5].

4 Examples

All the results were obtained with the own-developed codes. Here we present simple example of the flow in the cube in 3D, the simulation was made for the mixture of the dry air and the water steam. All the used constants and input data are given in SI units. For this special case we used the constants $\sigma_C = 1/1.3$,

	dry air	water steam
$c_p, JK^{-1}mol^{-1}$	1004	1911
$c_v, JK^{-1}mol^{-1}$	712	1450
$\gamma = \frac{c_p}{c_v}$	1.401123	1.317931
$R = c_p - c_v, JK^{-1}mol^{-1}$	292	461

The initial condition was formed by the whole area filled with the dry air, velocity regime $v = (15 m s^{-1}, 0 m s^{-1}, 10 m s^{-1})$.

At the inlet we consider conservation of the total quantities $\theta_0 = 273.15\text{ K}$, $p_0 = 101325\text{ Pa}$, and the velocity direction $\mathbf{d} = (15, 0, 10)$. At the outlet part we preferred the average pressure $p = 101115.15\text{ Pa}$. At the chosen part of the inlet (left) boundary we applied the maximal concentration ($=1$) of the added gas specie (water steam). This source of admixture flows into the area and dissipates. The computational mesh and resulting isolines of mixture concentration can be seen in figure 2, the figure 3 shows the isosurfaces of density.

Fig. 2. The passive mixture simulation, used mesh and concentration of added gas component.

Fig. 3. The passive mixture simulation, isolines of density.

Another example simulates the emission of gas with enhanced total quantities into the area. We simulate the injected gas with the total pressure $p_o = 101325 + 12882.888\text{ Pa}$, total density $\rho_o = 2.4955963\text{ kg m}^{-3}$, and properties $R_1 = 287.3\text{ J K}^{-1}\text{ mol}^{-1}$, $\gamma_1 = 1.3018$, gas is emitted through the chosen part of the inlet boundary. The initial condition was formed by the whole area filled with air, velocity regime 15 m s^{-1} . The simulation was made in 2D, figure 4 demonstrates the density evolution in time.

Fig. 4. The passive mixture simulation, isolines of density.

Conclusion

This paper shows the formulation of the equations describing the mixture of two inert perfect gases in 3D. The numerical method (finite volume method) is applied for the solution of these equations. Own software was programmed. The modification of the Riemann problem is used at the boundaries.

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