The simulation of the atmospheric flow with emmisions

Martin Kyncl[1,*] and *Jaroslav* Pelant[1,**]

[1]VZLÚ - Czech Aerospace Research Centre, Beranových 130, 199 05 Praha - Letňany, Czech Republic

Abstract. The aim of this work is to simulate the flow of the passive gas mixture and estimate the resulting concentration of the potentionally dangerous pollutant emmisions. We assume non-stationary compressible gas flow in the gravitational field described by the system of the RANS equations, equipped with the equation for the concentration of additional specie. Due to gravitational force effect we modify the boundary conditions and data resulting admissible situations. The real simulations of the atmospheric flow require the use of the wall functions for the boundary condition simulating the ground surface with given roughness. We show the modification of such wall functions. The computational results are obtained with the own-developed CFD code for the compressible turbulent mixture flow. The originality of this work lies with the special handling of the boundary conditions, and own computational code.

1 Introduction

The main topic 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-ω 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. The expected result is to construct a method for the estimates of the pollutant concentrations in the case of a sudden leakage of the substances hazardous to health. This contribution follows previous work [1–3].

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 $\Omega \in \boldsymbol{R}^N$, and time interval $(0, T)$, with $T > 0$. The system of the Reynolds-Averaged Navier-Stokes equations in 3D has the form

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

Here x_1, x_2, x_3 are the space coordinates, t the time, $\boldsymbol{w} = \boldsymbol{w}(x,t) = (\varrho, \varrho v_1, \varrho v_2, \varrho v_3, E)^T$ is the state vector, $\boldsymbol{f}_s = (\varrho v_s, \varrho v_s v_1 + \delta_{s1}p, \varrho v_s v_2 + \delta_{s2}p, \varrho v_s v_3 + \delta_{s3}p, (E+p)\,v_s)^T$ are the inviscid fluxes, $\boldsymbol{R}_s = (0, \tau_{s1}, \tau_{s2}, \tau_{s3}, \sum_{r=1}^{3}\tau_{sr}v_r + C_k\partial\theta/\partial x_s)^T$ are the viscous fluxes, $\boldsymbol{S}$ are additional sources. $\boldsymbol{v} = (v_1, v_2, v_3)^T$ denotes the velocity vector, ϱ is the density, p the pressure, θ the absolute temperature, $E = \varrho e + \frac{1}{2}\varrho\boldsymbol{v}^2$ the total energy. Further $\tau_{ij} = (\mu+\mu_T)S_{ij} - \delta_{ij}\frac{2}{3}\varrho k$, with $S_{11} = \frac{2}{3}\left(2\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3}\right), S_{12} = \frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}, S_{13} = \frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1}, S_{21} = S_{12}, S_{22} = \frac{2}{3}\left(-\frac{\partial v_1}{\partial x_1} + 2\frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3}\right), S_{23} = \frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2}, S_{31} = S_{13}, S_{32} = S_{23}, S_{33} = \frac{2}{3}\left(-\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} + 2\frac{\partial v_3}{\partial x_3}\right)$, 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 $C_k = (\frac{\mu}{P_r} + \frac{\mu_T}{P_{r_T}})c_v\gamma$, and P_r is laminar and P_{r_T} is turbulent Prandtl constant number. In our application of flow in the gravitational field we set the source terms to $\boldsymbol{S} = (0, \varrho g_1, \varrho g_2, \varrho g_3, \varrho\boldsymbol{g}\cdot\boldsymbol{v})$, where $\boldsymbol{g} = (g_1, g_2, g_3)$ 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 mollar mass of the ith 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)

$$\varrho c_p = \sum \varrho_i c_{pi}, \quad \varrho c_V = \sum \varrho_i c_{Vi},$$

*e-mail: kyncl@vzlu.cz
**e-mail: pelant@vzlu.cz

© The Authors, published by EDP Sciences. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (http://creativecommons.org/licenses/by/4.0/).

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

$$\gamma = \frac{c_p}{c_V} = \frac{\sum Y_i c_{pi}}{\sum Y_i c_{Vi}}.$$

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 [7]. The effective turbulent viscosity is $\mu_T = \varrho k/\omega$.

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

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

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

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

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 [8, 9]. We use either explicit or implicit finite volume method (FVM) to solve the systems sequentionally. Other possible discretizations were shown in [17, 18]. Here we present the discretization of the system (1) using FVM. By Ω_h let us the 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 $J \subset Z^+ = \{0, 1, \ldots\}$ 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 $\boldsymbol{n}_{ij}$ let us denote the unit outer normal to ∂D_i on Γ_{ij}. Let us construct a partition $0 = t_0 < t_1 < \ldots$ 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.

$$\int_{D_i}\int_{t_k}^{t_{k+1}} \frac{\partial \boldsymbol{w}}{\partial t} dx\, dt + \int_{t_k}^{t_{k+1}}\int_{D_i} \sum_{s=1}^{3} \frac{\partial \boldsymbol{f}_s(\boldsymbol{w})}{\partial x_s} dx\, dt = \int_{t_k}^{t_{k+1}}\int_{D_i} \sum_{s=1}^{3} \frac{\partial \boldsymbol{R}_s(\boldsymbol{w}, \nabla \boldsymbol{w})}{\partial x_s} dx\, dt \quad (6)$$

Using the Green's theorem on D_i it is

$$\int_{D_i} \sum_{s=1}^{3} \frac{\partial \boldsymbol{f}_s(\boldsymbol{w})}{\partial x_s} dx = \int_{\partial D_i} \sum_{s=1}^{3} \boldsymbol{f}_s(\boldsymbol{w}) n_s\, dS, \quad (7)$$

$$\int_{D_i} \sum_{s=1}^{3} \frac{\partial \boldsymbol{R}_s(\boldsymbol{w}, \nabla \boldsymbol{w})}{\partial x_s} dx = \int_{\partial D_i} \sum_{s=1}^{3} \boldsymbol{R}_s(\boldsymbol{w}, \nabla \boldsymbol{w}) n_s\, dS.$$

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

$$\int_{D_i} (\boldsymbol{w}(x, t_{k+1}) - \boldsymbol{w}(x, t_k))\, dx + \int_{t_k}^{t_{k+1}} \sum_{\Gamma_{ij}\in\Gamma_{D_i}} \int_{\Gamma_{ij}} \sum_{s=1}^{3} (\boldsymbol{f}_s(\boldsymbol{w}) - \boldsymbol{R}_s(\boldsymbol{w}, \nabla \boldsymbol{w}))\,(n_{ij})_s\, dS\, dt = 0 \quad (8)$$

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

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

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

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

with $\boldsymbol{w}_i^l$, $\boldsymbol{w}_j^l$ 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 $\boldsymbol{w}_j^l$ has to be specified. Here we show the numerical flux based on the solution of the Riemann problem for the split Euler equations. By $\boldsymbol{w}_{\Gamma_{ij}}^l$ let us denote the state vector $\boldsymbol{w}$ at the center of the edge Γ_{ij} at the time instant t_l, and let us suppose $\boldsymbol{w}_{\Gamma_{ij}}^l$ 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

$$\int_{\Gamma_{ij}} \sum_{s=1}^{3} \boldsymbol{f}_s(\boldsymbol{w}(x,t_l))(n_{ij})_s \, dS \approx |\Gamma_{ij}| \sum_{s=1}^{3} \boldsymbol{f}_s(\boldsymbol{w}_{\Gamma_{ij}}^l)(n_{ij})_s, \tag{10}$$

$$\int_{\Gamma_{ij}} \sum_{s=1}^{3} \boldsymbol{R}_s(\boldsymbol{w}(x,t_l), \nabla\boldsymbol{w}(x,t_l))(n_{ij})_s \, dS \approx$$

$$|\Gamma_{ij}| \sum_{s=1}^{3} \boldsymbol{R}_s(\boldsymbol{w}_{\Gamma_{ij}}^l, \nabla\boldsymbol{w}_{\Gamma_{ij}}^l)(n_{ij})_s.$$

Here $\nabla\boldsymbol{w}_{\Gamma_{ij}}^l$ denotes the $\nabla\boldsymbol{w}$ 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

$$(\boldsymbol{w}_i^{k+1} - \boldsymbol{w}_i^k) \quad + \quad \Phi(\boldsymbol{w}_i^k) = 0, \tag{11}$$

with

$$\Phi(\boldsymbol{w}_i^k) = \frac{\tau_k}{|D_i|} \sum_{\Gamma_{ij}\in\Gamma_{D_i}} |\Gamma_{ij}| \left(\boldsymbol{H}(\boldsymbol{w}_i^k, \boldsymbol{w}_j^k, \boldsymbol{n}_{ij}) - \sum_{s=1}^{3} \boldsymbol{R}_s(\boldsymbol{w}_{\Gamma_{ij}}^k, \nabla\boldsymbol{w}_{\Gamma_{ij}}^k) n_s \right).$$

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 $\boldsymbol{w}_{\Gamma_{ij}}^k$ 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 [10]. The crucial problem of this discretization lies with the evaluation of the edge values $\boldsymbol{w}_{\Gamma_{ij}}^k$. Or one deals with the problem of finding the face fluxes $\boldsymbol{H}(\boldsymbol{w}_i^k, \boldsymbol{w}_j^k, \boldsymbol{n}_{ij})$. It is also possible to use the **implicit scheme**

$$(\boldsymbol{w}_i^{k+1} - \boldsymbol{w}_i^k) \quad + \quad \Phi(\boldsymbol{w}_i^{k+1}) = 0. \tag{12}$$

The Newton method.
We may proceed as shown in [10][page 216]. At each time level t_{k+1} the following iterative scheme is applied:

$$\boldsymbol{w}_i^{k+1,0} = \boldsymbol{w}_i^k \tag{13}$$

$$\left(\mathbb{I} + \frac{D\Phi(\boldsymbol{w}_i^{k+1,r})}{D\boldsymbol{w}} \right) (\boldsymbol{w}_i^{k+1,r+1} - \boldsymbol{w}_i^{k+1,r}) = \tag{14}$$

$$-\boldsymbol{w}_i^{k+1,r} + \boldsymbol{w}_i^k - \Phi(\boldsymbol{w}_i^{k+1,r}), \quad r = 0, 1, \ldots$$

Here $\frac{D\Phi(\boldsymbol{w})}{D\boldsymbol{w}}$ is the Jacobian matrix of the mapping Φ. Using such process we obtain the sequence $\left\{\boldsymbol{w}_i^{k+1,r}\right\}$ converging to $\boldsymbol{w}_i^{k+1}$ as $r \to \infty$.

The crucial problem of this discretization lies with the evaluation of the face fluxes $\boldsymbol{H}(\boldsymbol{w}_i^{k+1}, \boldsymbol{w}_j^{k+1}, \boldsymbol{n}_{ij})$. One possibility is to use the linearization via the Taylor expansion of the vector function $\boldsymbol{H}(\boldsymbol{wI}, \boldsymbol{wJ}, \boldsymbol{n})$, this was shown in [8].

3.1 The gas mixture equations discretization

As noted before, we will solve the system (1) and the equation (2) sequentially at each time instant. In order to determine the unknown mass fraction Y_1 we consider the following system

$$\frac{\partial w}{\partial t} + \sum_{s=1}^{3} \frac{\partial f_s(w)}{\partial x_s} = \sum_{s=1}^{3} \frac{\partial \boldsymbol{R}_s(w, \nabla w)}{\partial x_s} + s(w) \quad \text{in } Q_T. \tag{15}$$

Here

$$w = \varrho Y_1, f_s = \varrho Y_1 v_s, \boldsymbol{R}_s = \sigma_C \mu_T \frac{\partial Y_1}{\partial x_s}, s(w) = 0.$$

Using the FVM discretization, shown above, we obtain the following implicit scheme for the unknown $\Delta w = w|^{n+1} - w|^n$ at each time instant t_n

$$\left(\frac{|D_i|}{\tau_n} + \sum_{\Gamma_{ij}\in\Gamma_{D_i}} |\Gamma_{ij}| \left. \frac{\partial(H-\mathcal{R})}{\partial wI} \right|_{ij}^{n} \right) \Delta\boldsymbol{w}_i + \tag{16}$$

$$+ \sum_{\Gamma_{ij}\in\Gamma_{D_i}} |\Gamma_{ij}| \left. \frac{\partial(H-\mathcal{R})}{\partial wJ} \right|_{ij}^{n} \Delta\boldsymbol{w}_j = - \sum_{\Gamma_{ij}\in\Gamma_{D_i}} |\Gamma_{ij}| \, (H-\mathcal{R})|_{ij}^{n}.$$

Here $H|_{ij}^n$ is the approximation of the fluxes $\sum_{s=1}^{3} f_s(w) n_{ij_s}|_{ij}^n$ through the face Γ_{ij} at time instant t_k. Using the Vijayasundaram flux we can approximate these fluxes as follows:

$$\left. \sum_{s=1}^{3} f_s(w) n_{ij_s} \right|_{ij}^{n} = \boldsymbol{v}\,|_{ij}^n \cdot \boldsymbol{n}_{ij}\, w|_{ij}^n \approx H|_{ij}^n$$

$$H|_{ij}^n = H(w_i^n, w_j^n, \boldsymbol{n}_{ij}) = a^+ w_i^n + a^- w_j^n,$$

where $a^+ = max(\boldsymbol{v}|_{ij}^n \cdot \boldsymbol{n}_{ij}, 0)$, $a^- = min(\boldsymbol{v}|_{ij}^n \cdot \boldsymbol{n}_{ij}, 0)$ are computed constants. The values $\boldsymbol{v}|_{ij}^n$ are either known (from the Riemann flux across the face Γ_{ij}), or we can choose $\boldsymbol{v}|_{ij}^n = (\boldsymbol{v}|_{D_i} + \boldsymbol{v}|_{D_j})/2$. The Jacobians of such mapping $H(wI, wJ, n_{ij})$ are

$$\frac{\partial H}{\partial wI} = a^+, \quad \frac{\partial H}{\partial wJ} = a^-.$$

The symbol $\mathcal{R}$ denotes the approximation of the viscous flux $\sum_{s=1}^{3} \boldsymbol{R}_s(w, \nabla w)(\boldsymbol{n}_{ij})_s$. By $\left.\frac{\partial\mathcal{R}}{Dwl}\right|_{ij}^n$, $\left.\frac{\partial\mathcal{R}}{\partial wJ}\right|_{ij}^n$ we mean the Jacobian of the mapping $\mathcal{R}(wI, wJ, ...)$ dependent on the states wI, wJ at the neighbouring elements over the face Γ_{ij}

$$\sum_{s=1}^{3} \boldsymbol{R}_s(w|_{ij}^n, (\nabla w)|_{ij}^n)(\boldsymbol{n}_{ij})_s = \sigma_C \mu_T |_{ij}^n \nabla Y_1|_{ij}^n \cdot \boldsymbol{n}_{ij} \approx \mathcal{R}|_{ij}^n$$

$$\mathcal{R}|_{ij}^{n} = \sigma_C \widetilde{\mu_T} \widetilde{\nabla Y_1} \cdot \boldsymbol{n}_{ij}$$

$$\left.\frac{\partial \mathcal{R}}{\partial w I}\right|_{ij}^{n} = \left.\left(\sigma_C \widetilde{\mu_T} \frac{\partial}{\partial w I} (\widetilde{\nabla Y_1} \cdot \boldsymbol{n}_{ij})\right)\right|_{ij}^{n}$$

Here $\widetilde{\mu_T}$ is the approximation (known constant) of the viscosity $\mu_T|_{ij}^n$ at the face Γ_{ij} at time instant t_n. The gradient $\nabla Y_1|_{ij}^n$ at the face Γ_{ij} can be approximated as $\widetilde{\nabla Y_1}$, using the m-point rule.
The system (16) can be written in a matrix form

$$\mathbb{A}_{Y_1} \Delta \boldsymbol{w} = \boldsymbol{b}, \tag{17}$$

with

$$\Delta \boldsymbol{w} = (\Delta w_1, \Delta w_2, \ldots, \Delta w_n)^T,$$

$$\boldsymbol{b} = (b_1, \ldots, b_n)^T,$$

$$b_i = -\sum_{\Gamma_{il} \in \Gamma_{D_i}} |\Gamma_{il}| \, (H - \mathcal{R})|_{il}^{n} \;, i = 1, \ldots, n,$$

and $\mathbb{A}_Y$ is the matrix with

$$a_{ij} = \begin{cases} \frac{|D_i|}{\tau_k} + \sum_{l \in \Gamma_{D_i}} |\Gamma_{il}| \, \frac{\partial (H-\mathcal{R})}{\partial w I}\Big|_{il}^{n}, & i = j, \\ |\Gamma_{ij}| \, \frac{\partial (H-\mathcal{R})}{\partial w J}\Big|_{ij}^{n}, & i \neq j, \; j \in S(i), \\ 0, & i \neq j, \; j \notin S(i). \end{cases}$$

We use the GMRES method with the ILUK preconditioning in order to solve this system.

4 Boundary conditions

In order to to get the state variables at each boundary face we solve the local boundary problem with the use the original analysis of exact solution of the Riemann problem. This approach was shown and described in [4, 16] and analyzed also in [9], [13]. Using the thorough analysis of the Riemann problem we have shown, that the RIC for the local problem can be partially replaced by the suitable complementary conditions. We suggest such complementary conditions accordingly to the desired preference. This way it is possible to construct the boundary conditions by the preference of total values, by preference of pressure, velocity, mass flow, temperature. Further, using the suitable complementary conditions, it is possible to simulate the flow in the vicinity of the diffusible barrier. On the contrary to the initial-value Riemann problem, the solution of such modified problems can be written in the closed form for some cases. Moreover, using such construction, the local conservation laws are not violated.

4.1 Wall functions

In the case of the coarse mesh with the first cell in the log layer we use the so-called wall functions for the values inside the first cell.
Standard wall functions
We estimate the friction velocity u_τ, assuming the law of the wall (see [3, 7]) to be valid at the closest volume, i.e. solve the implicit equation

$$U_P = u_\tau \left[\frac{1}{\kappa} ln(u_\tau y_P \varrho_w / \mu_w) + C \right].$$

The wall friction $\tau_w = \mu \frac{\partial U}{\partial y}|_w$ is then estimated as $\tau_w = \varrho_w u_\tau^2$. Measurements indicate $C \approx 5.0$ for smooth surfaces, $\kappa \approx 0.41$ (Karman's constant), y_P denotes the distance from surface (of the first cell). For the rough surface, with elements of average height k_S, experiments show that the C is a function of k_S,

$$C \to 8.5 - \frac{1}{\kappa} ln \, k_S^+, \text{ where } \quad k_S^+ = \frac{u_\tau \varrho_w}{\mu_w} k_S .$$

Here k_S^+ is dimensionless roughness height.

The momentum equations are solved with the modified effective viscosity μ_e at the wall: $\mu_e \frac{U_P}{y_P} = \tau_w$. The values for the k, ω at the first cell are set using log layer equations

$$\mu_e = \frac{\varrho_w u_\tau y_P}{\left[\frac{1}{\kappa} ln(u_\tau y_P \varrho_w / \mu_w) + C\right]}, \; k_P = \frac{u_\tau^2}{\sqrt{\beta^*}}, \; \omega_P = \frac{u_\tau}{\sqrt{\beta^*} \kappa y_P}.$$

The main drawback of this simple wall function are the cases with separated flow where $\tau_w \to 0$, consequently giving $k_p \to 0$.

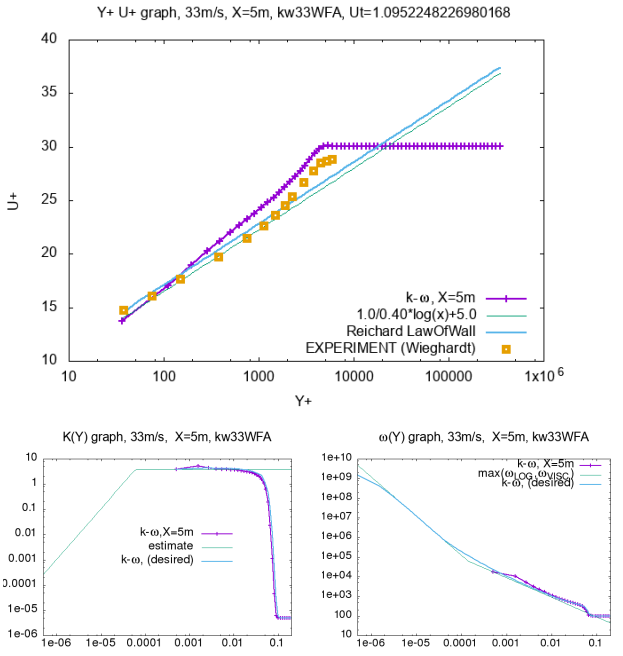

Fig. 1. CFD simulations, standard wall function, height of the first cell 0.001m, regime U_∞ =33 m.s^{-1}. Graph for the $U+$ (comparison with experimantal data), $k(Y), \omega(Y)$ in the vertical cut at x=5m.

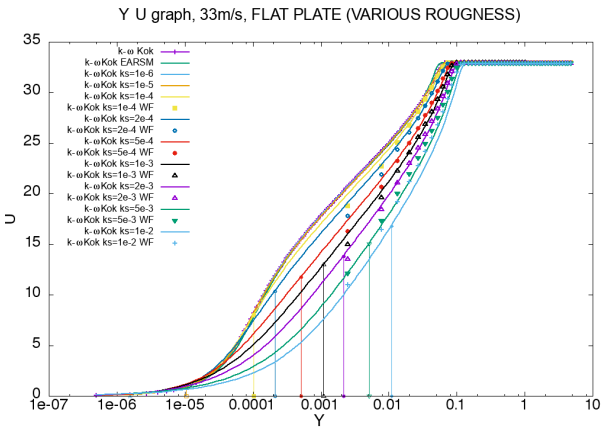

Fig. 2. CFD simulations, standard wall function over rough surfaces, height of the first cell 0.001m, regime U_∞ =33 m.s^{-1}. Graph for the U, k, ω in the vertical cut at x=5m (comparison with expected data).

Launder-Spalding/Chieng-Launder methodology

Estimate the friction velocity using the known value k_P at the first cell: $(u_\tau^*)^2 = k_P\sqrt{\beta^*}$, then estimate shear stress τ_w using modified log layer equation

$$\tau_w = \frac{\varrho_w u_\tau^* U_P}{\frac{1}{\kappa} ln(u_\tau^* y_P \varrho_w/\mu_w) + C}.$$

The momentum equations are solved with the modified effective viscosity μ_e at the wall: $\mu_e \frac{U_P}{y_P} = \tau_w$, i.e.

$$\mu_e = \frac{\varrho_w u_\tau^* y_P}{\frac{1}{\kappa} ln(u_\tau^* y_P \varrho_w/\mu_w) + C}.$$

Further, the production term $P_k = \tau_w \frac{\partial U}{\partial y}$ (in the log layer) can be estimated as

$$P_k = \frac{\tau_w^2}{\kappa \varrho_w u_\tau^* y}.$$

Integrating over the log layer in the first cell (height y_N), the average value at this cell is then estimated

$$\overline{P_k} = \frac{1}{y_N}\int_0^{y_N} P_k dy = \frac{\tau_w^2}{\kappa \varrho_w u_\tau^* y_N} ln\left(\frac{y_N}{y_V}\right).$$

Here y_V is the sublayer thickness, typically set such that $y_V\sqrt{k_P}\varrho_w/\mu_w = 20$. We use other estimate $y_V = \frac{2\mu_w \kappa}{u_\tau \sqrt{\beta^*}\varrho_w}$. The average dissipation term $\overline{\beta^*\omega k}$ at the near-wall cell is then estimated using viscous and log layer approximations for k, ω

$$\text{(viscous sublayer)} \quad k = \frac{k_P}{y_V^2} y^2, \quad \beta^* y^2 \omega \varrho_w/\mu_w = 2$$

$$\text{(log layer)} \quad k = \frac{u_\tau^2}{\sqrt{\beta^*}}, \quad \omega = \frac{u_\tau}{\sqrt{\beta^*}\kappa y}$$

$$\overline{\beta^*\omega k} = \frac{1}{y_N}\int_0^{y_N} \beta^*\omega k \; dy = \frac{1}{y_N}\left[\frac{2\mu_w k_P}{\varrho_w y_V} + \frac{u_\tau^{*3}}{\kappa} log(\frac{y_N}{y_V})\right].$$

Then solve the turbulent kinetic energy with modified integrated production terms. At last set ω at the first cell as

$$\omega_P = \frac{u_\tau}{\sqrt{\beta^*}\kappa y_P}.$$

Another modification is to set average omega production $\overline{P_\omega}$ at the first cell as

$$\overline{P_\omega} = \alpha_\omega \overline{P_k}\omega/k. \tag{18}$$

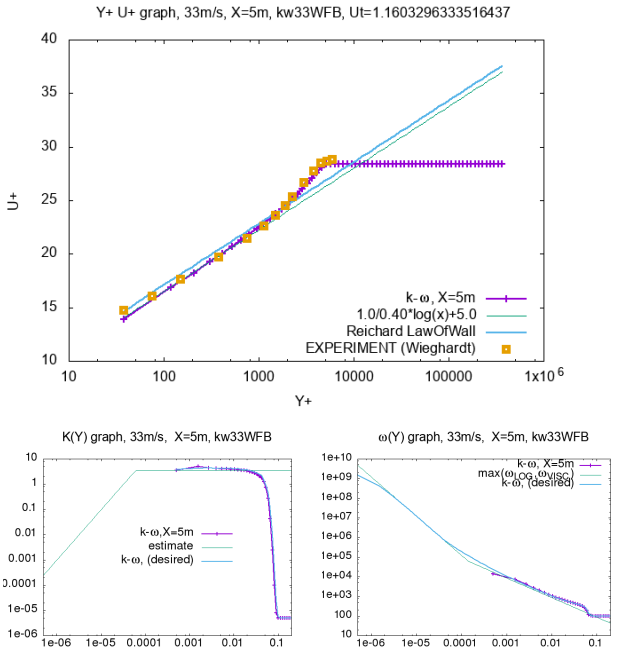

Fig. 3. CFD simulations, Launder-Spalding/Chieng-Launder methodology, height of the first cell 0.001m, regime U_∞ =33 m.s^{-1}. Graph for the $U+$ (comparison with experimantal data), $k(Y), \omega(Y)$ in the vertical cut at x=5m.

5 Examples

All the results and mesh were obtained with the own-developed codes. The aim of the following computations was to achieve relatively quickly some estimate of the gas dispersion in the case of some possibly dangerous pollution. Let the surface data be given by a set of point coordinates (left picture) and scaled. Then the surface mesh is constructed, and volumes created using own softwar. Computation run with the initial condition with the total quantities $\theta_0 = 273.15\ K$, $p_0 = 101325\ Pa$, and regime velocity $v_1 = 5\ m\ s^{-1}$, and fixed emission source located at the chosen point. The figure 4 shows the simulation of the gas mixture flow over such simple terrain.

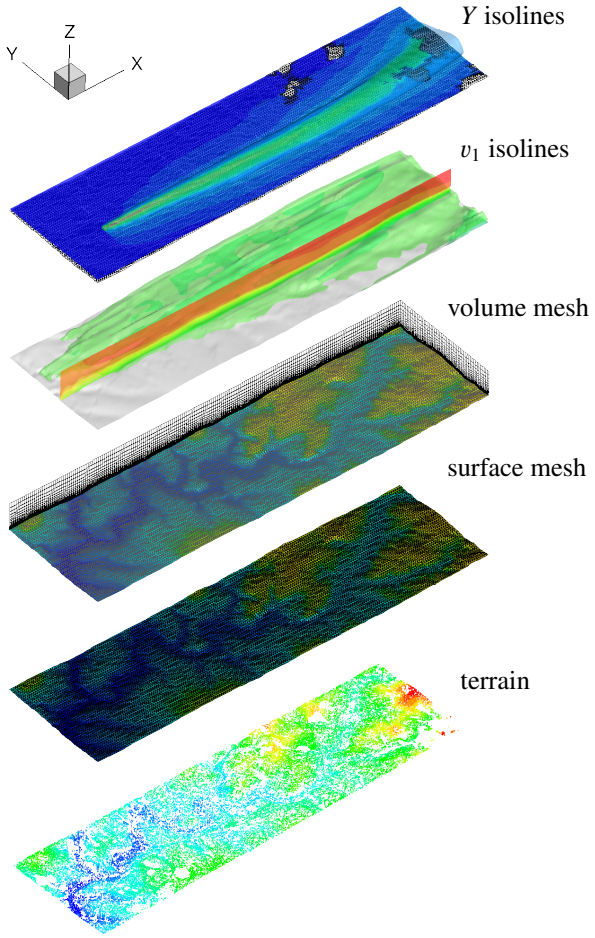

Fig. 4. The simulation of the flow over the terrain: (from bottom) set of points, surface mesh, volume mesh, isolines of velocity, isolines of the mass fraction Y.

Conclusion

This paper is focused on the numerical simulation of the mixture of two inert perfect gases in 3D. The finite volume method is applied for the solution of the system of equations. The modification of the Riemann problem and its solution was used at the boundaries. All codes were implemented into the own-developed software. The numerical examples were presented. The original intention was to use the modified software for the quick estimation of the gaseous pollution of the air. This may be critical in the case of the sudden leakage of the substances hazardous to health. The estimates computed with this software are undoubtedly more precise than a simple set of concentric circles. Further development and comparison with the experimental data (from the wind tunnel) is still in the process.

The results originated with the support of Ministry of the Interior of the Czech Republic, project VI20172020092, project SCENT, Grant MSM 0001066902 of the Ministry of Education of the Czech Republic, and Ministry of Industry and Trade of the Czech Republic for the long-term strategic development of the research organization. The authors acknowledge this support.

References

1. M. Kyncl and J. Pelant, *EPJ WoC*, **114**, 02064, (2016)
2. M. Kyncl and J. Pelant, *ENGINEERING MECHANICS 2016*, **22**, p.367-370, (2016)
3. M. Kyncl and J. Pelant, *EPJ WoC*, **92**, 02044, (2015)
4. M. Kyncl and J. Pelant, *EPJ WoC*, **143**, 02061, (2017)
5. M. Kyncl and J. Pelant, *ENGINEERING MECHANICS 2018*, **24**, p.469-472, (2018)
6. Reynolds, A. J., *J. Mech. Eng. Sci.*, **11**, p. 290–294, (1969)
7. C. J. Kok, *AIAA Journal*, **38**, 7, (2000)
8. M. Kyncl and J. Pelant, *Implicit method for the 3d RANS equations with the k-ω (Kok) Turbulent Model.* Technical report R5453, (2012)
9. M. Kyncl and J. Pelant, *Implicit method for the 3d Euler equations.* Technical report R5375, VZLÚ, (2012)
10. M. Feistauer, J. Felcman, and I. Straškraba, *Mathematical and Computational Methods for Compressible Flow*. Oxford University Press, Oxford, (2003)
11. M. Feistauer, *Mathematical Methods in Fluid Dynamics*. Longman Scientific & Technical, Harlow, (1993)
12. E. F. Toro, *Riemann Solvers and Numerical Methods for Fluid Dynamics*. Springer, Berlin, (1997)
13. M. Kyncl. *Numerical solution of the three-dimensional compressible flow.* Doctoral Thesis, Prague, (2011)
14. M. Kyncl and J. Pelant, *Proc. ECCOMAS 2014, ECFD VI, 20.-25.7.2014*, Spain (2014)
15. M. Kyncl and J. Pelant, *Appl. Mech. and Mat.*, **821**, 70-78, (2016)
16. M. Kyncl and J. Pelant, *Proc. ECCOMAS 2016, 5.-10.6.2016*, Greece (2016)
17. J. Česenek, *EPJ WoC* **114**, 02012 (2016)
18. J. Česenek, *EPJ WoC* **180**, 02016 (2018)