

Numerical simulation of the passive gas mixture flow

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Abstract. The aim of this paper is the numerical solution of the equations describing the non-stationary compressible turbulent multicomponent flow in gravitational field. The mixture of perfect inert gases is assumed. We work with the RANS equations equipped with the k-omega and the EARSM turbulence models. For the simulation of the wall roughness we use the modification of the specific turbulent dissipation. The finite volume method is used, with thermodynamic constants being functions in time and space. In order to compute the fluxes through the boundary faces we use the modification of the Riemann solver, which is the original result. We present the computational results, computed with the own-developed code (C, FORTRAN, multiprocessor, unstructured meshes in general).

1 Introduction

The aim of this work is to simulate the 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. We choose the well-known finite volume method to discretize the analytical problem, represented by the system of the equations in generalized (integral) form. In order to apply this method we split the area of the interest into the elements, and we construct a piecewise constant solution in time. The crucial problem of this method lies in the evaluation of the so-called fluxes through the edges/faces of the particular elements. We use the analysis of the exact solution of the Riemann problem for the discretization of the fluxes through the boundary edges/faces. Own algorithms for the solution of the boundary problem were coded, and used in the numerical examples.

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, $\mathbf{R}_s = (0, \tau_{s1}, \tau_{s2}, \tau_{s3}, \sum_{r=1}^3 \tau_{sr} v_r + C_k \theta \delta / \partial x_s)^T$ 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, $E = \varrho e + \frac{1}{2} \varrho \mathbf{v}^2 + \varrho k$ 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 $S_{11} = \frac{2}{3} \left(2 \frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3} \right)$, $S_{12} = \frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}$, $S_{13} = \frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1}$, $S_{21} = S_{12}$, $S_{22} = \frac{2}{3} \left(-\frac{\partial v_1}{\partial x_1} + 2 \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3} \right)$, $S_{23} = \frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2}$, $S_{31} = S_{13}$, $S_{32} = S_{23}$, $S_{33} = \frac{2}{3} \left(-\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} + 2 \frac{\partial v_3}{\partial x_3} \right)$, 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 $C_k = \left(\frac{\mu}{P_r} + \frac{\mu_T}{P_{rT}} \right) c_v \gamma$, 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

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the species mass fractions Y_1, Y_2 , with $Y_1 = \frac{\rho_1}{\rho}, Y_2 = \frac{\rho_2}{\rho}$, it is $Y_1 + Y_2 = 1$. The thermodynamic constants of the mixture satisfy (using the decomposition of the internal specific energy and enthalpy)

$$\rho c_p = \sum \rho_i c_{pi}, \quad \rho c_v = \sum \rho_i c_{vi},$$

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

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

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

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

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 $\mu_T = \rho k / \omega$.

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

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

where k the specific 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

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

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 $\bar{\Omega}_h = \bigcup_{i \in J} D_i$. 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.

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

Using the Green's theorem on D_i it is

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

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)

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

We define a finite volume approximate solution of the system studied (1) as a piecewise constant vector-valued functions \mathbf{w}_h^k , $k = 0, 1, \dots$, 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

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

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 $\mathbf{w}_{\Gamma_{ij}}^l$ let us denote the state vector \mathbf{w} at the center of the edge Γ_{ij} at the time instant t_l , and let us suppose $\mathbf{w}_{\Gamma_{ij}}^l$ 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

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

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

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

$$\frac{|D_i|}{\tau_k} (\mathbf{w}_i^{k+1} - \mathbf{w}_i^k) + \sum_{\Gamma_{ij} \in \Gamma_{D_i}} |\Gamma_{ij}| \sum_{s=1}^3 (\mathbf{f}_s(\mathbf{w}_{\Gamma_{ij}}^k) n_s - \mathbf{R}_s(\mathbf{w}_{\Gamma_{ij}}^k, \nabla \mathbf{w}_{\Gamma_{ij}}^k) n_s) = 0 \quad (11)$$

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 $\mathbf{w}_{\Gamma_{ij}}^k$ 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 $\mathbf{w}_{\Gamma_{ij}}^k$. Or one deals with the problem of finding the face fluxes $\mathbf{H}(\mathbf{w}_i^k, \mathbf{w}_j^k, \mathbf{n}_{ij})$. It is also possible to use the **implicit scheme**

$$\frac{|D_i|}{\tau_k} (\mathbf{w}_i^{k+1} - \mathbf{w}_i^k) + \sum_{\Gamma_{ij} \in \Gamma_{D_i}} |\Gamma_{ij}| \left(\mathbf{H}(\mathbf{w}_i^{k+1}, \mathbf{w}_j^{k+1}, \mathbf{n}_{ij}) - \sum_{s=1}^3 \mathbf{R}_s(\mathbf{w}_{\Gamma_{ij}}^{k+1}, \nabla \mathbf{w}_{\Gamma_{ij}}^{k+1}) n_s \right) = 0 \quad (12)$$

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

$$\mathbf{H}_{ij}^k = \sum_{s=1}^3 \mathbf{f}_s(\mathbf{w}_{\Gamma_{ij}}^k)(n_{ij})_s. \quad (13)$$

To approximate the face values $\mathbf{w}_{\Gamma_{ij}}^k$ 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 \mathbf{w}_i^k and \mathbf{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 $\mathbf{n} = (n_1, n_2, n_3)$, given by the face normal $\mathbf{n} = \mathbf{n}_{ij}$.

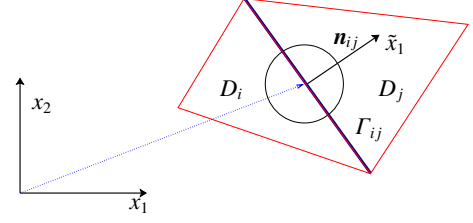


Fig. 1. Coordinate transformation for the inner edges in 2D.

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]:

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

The values \mathbf{w}_i^k and \mathbf{w}_j^k adjacent to the face Γ_{ij} are known, forming the initial conditions

$$\mathbf{q}(\tilde{x}_1, 0) = \mathbf{q}_L = \mathbb{Q} \mathbf{w}_i^k, \quad \tilde{x}_1 < 0, \quad (15)$$

$$\mathbf{q}(\tilde{x}_1, 0) = \mathbf{q}_R = \mathbb{Q} \mathbf{w}_j^k, \quad \tilde{x}_1 > 0. \quad (16)$$

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 $\mathbf{q}_{RS}(\mathbf{q}_L, \mathbf{q}_R, \tilde{x}_1, t)$ 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 $\mathbf{q}_{\Gamma_{ij}} = \mathbf{q}_{RS}(\mathbf{q}_L, \mathbf{q}_R, 0, t)$. The backward transformation of the state vector $\mathbf{q}_{\Gamma_{ij}}$ into the global coordinates is

$$\mathbf{w}_{\Gamma_{ij}}^k = \mathbb{Q}^{-1} \mathbf{q}_{\Gamma_{ij}} = \mathbb{Q}^{-1} \mathbf{q}_{RS}(\mathbb{Q} \mathbf{w}_i^k, \mathbb{Q} \mathbf{w}_j^k, 0, t). \quad (17)$$

The constructed numerical flux can be written as

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

Let Γ_{ij} be the face of the element D_i laying at the boundary of the computational area. To approximate the face values $\mathbf{w}_{\Gamma_{ij}}^k$ at time instant t_k we solve the incomplete simplified system (19) in the vicinity of the face Γ_{ij} in time with the initial condition (20) determined by the state vector \mathbf{w}_i^k . By adding properly chosen equations into the system (19),(20) it is possible to reconstruct the boundary state \mathbf{q}_B such that the system (19),(20) 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 The Riemann Problem for the Split Euler Equations

For many numerical methods dealing with the two or three dimensional equations, describing the compressible flow,

it is useful to solve the Riemann problem for the 3D split Euler equations. We search the solution of the system of partial differential equations in time t and space (x, y, z)

$$\begin{aligned} \frac{\partial \varrho}{\partial t} + \frac{\partial \varrho u}{\partial x} &= 0 \\ \frac{\partial \varrho u}{\partial t} + \frac{\partial (\varrho u^2 + p)}{\partial x} &= 0 \\ \frac{\partial \varrho v}{\partial t} + \frac{\partial \varrho u v}{\partial x} &= 0 \\ \frac{\partial \varrho w}{\partial t} + \frac{\partial \varrho u w}{\partial x} &= 0 \\ \frac{\partial E}{\partial t} + \frac{\partial u(E+p)}{\partial x} &= 0, \end{aligned} \quad (19)$$

equipped with the initial conditions

$$\varrho(x, t) = \varrho_L, \mathbf{v}(x, t) = \mathbf{v}_L, p(x, t) = p_L, \quad x < 0, \quad (20)$$

$$\varrho(x, t) = \varrho_R, \mathbf{v}(x, t) = \mathbf{v}_R, p(x, t) = p_R, \quad x > 0. \quad (21)$$

Vector $\mathbf{v} = (u, v, w)$ denotes the velocity, ϱ density, p pressure, $E = \varrho e + \varrho |\mathbf{v}|^2$ is the total energy, with e denoting the specific internal energy. We assume the equation of state for the calorically ideal gas

$$e = \frac{p}{\varrho(\gamma - 1)}.$$

‘Split’ means here that we still have 5 equations in 3D, but the dependence on y, z (space coordinates) is neglected, and we deal with the system for one space variable x . The system (19) is considered in the set $Q_\infty = (-\infty, \infty) \times (0, +\infty)$.

The solution of this problem is fundamentally the same as the solution of the Riemann problem for the 1D Euler equations, see [4, page 138]. In fact, the solution for the pressure, the first component of the velocity, and the density is exactly the same as in one-dimensional case. It is a characteristic feature of the hyperbolic equations, that there is a possible raise of discontinuities in solutions, even in the case when the initial conditions are smooth, see [8, page 390]. Here the concept of the classical solution is too restrictive, and therefore we seek a weak solution of this problem. To distinguish physically admissible solutions from nonphysical ones, entropy condition must be introduced, see [8, page 396]. By the solution of the problem (19),(20),(21) we mean the *weak entropy solution* of this problem in Q_∞ . The analysis to the solution of this problem can be found in many books, i.e. [4], [8], [9]. The general theorem on the solvability of the Riemann problem can be found in [4, page 88].

The solution is piecewise **smooth** and its general form can be seen in Fig. 2, where the system of half lines is drawn.

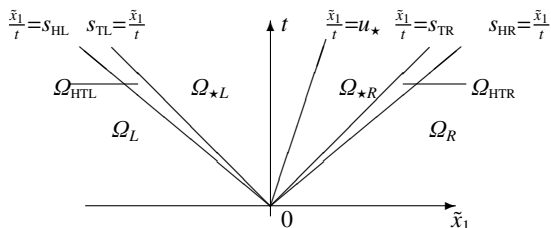


Fig. 2. Structure of the solution of the Riemann problem (19),(20),(21)

These half lines define regions, where solution is either constant or given by a smooth function. Let us define the open sets called **wedges** (see Fig. 2):

$$\begin{aligned} \Omega_L &= \text{wedge}(L_{-\infty}, s_{HL}), & \Omega_{*R} &= \text{wedge}(u_*, s_{TR}), \\ \Omega_{HTL} &= \text{wedge}(s_{HL}, s_{TL}), & \Omega_{HTR} &= \text{wedge}(s_{TR}, s_{HR}), \\ \Omega_{*L} &= \text{wedge}(s_{TL}, u_*), & \Omega_R &= \text{wedge}(s_{HR}, L_{+\infty}). \end{aligned}$$

Using the theory in [4], [8], [9], we can write the solution for the primitive variables as

$$\begin{aligned} (\varrho, u, v, w, p)|_{\Omega_L} &= (\varrho_L, u_L, v_L, w_L, p_L), \\ (\varrho, u, v, w, p)|_{\Omega_{*L}} &= (\varrho_{*L}, u_*, v_L, w_L, p_*), \\ (\varrho, u, v, w, p)|_{\Omega_{*R}} &= (\varrho_{*R}, u_*, v_R, w_R, p_*), \\ (\varrho, u, v, w, p)|_{\Omega_R} &= (\varrho_R, u_R, v_R, w_R, p_R). \end{aligned}$$

The following relations for these variables hold:

$$u_* = u_L + \begin{cases} -(p_* - p_L) \left(\frac{2}{p_* + \frac{\gamma-1}{\gamma+1} p_L} \right)^{\frac{1}{2}}, & p_* > p_L \\ \frac{2}{\gamma-1} a_L \left[1 - \left(\frac{p_*}{p_L} \right)^{(\gamma-1)/2\gamma} \right], & p_* \leq p_L \end{cases} \quad (22)$$

$$\varrho_{*L} = \begin{cases} \varrho_L \frac{\frac{\gamma-1}{\gamma+1} \frac{p_L}{p_*} + 1}{\frac{p_*}{p_L} + \frac{\gamma-1}{\gamma+1}}, & p_* > p_L \\ \varrho_L \left(\frac{p_*}{p_L} \right)^{\frac{1}{\gamma}}, & p_* \leq p_L \end{cases} \quad (23)$$

$$s_{TL}^1 = \begin{cases} u_L - a_L \sqrt{\frac{\gamma+1}{2\gamma} \frac{p_*}{p_L} + \frac{\gamma-1}{2\gamma}}, & p_* > p_L \\ u_* - a_L \left(\frac{p_*}{p_L} \right)^{(\gamma-1)/2\gamma}, & p_* \leq p_L \end{cases} \quad (24)$$

$$u_* = u_R + \begin{cases} (p_* - p_R) \left(\frac{2}{p_* + \frac{\gamma-1}{\gamma+1} p_R} \right)^{\frac{1}{2}}, & p_* > p_R, \\ -\frac{2}{\gamma-1} a_R \left[1 - \left(\frac{p_*}{p_R} \right)^{(\gamma-1)/2\gamma} \right], & p_* \leq p_R \end{cases} \quad (25)$$

$$\varrho_{*R} = \begin{cases} \varrho_R \frac{\frac{p_*}{p_R} + \frac{\gamma-1}{\gamma+1}}{\frac{\gamma-1}{\gamma+1} \frac{p_*}{p_R} + 1}, & p_* > p_R \\ \varrho_R \left(\frac{p_*}{p_R} \right)^{\frac{1}{\gamma}}, & p_* \leq p_R \end{cases} \quad (26)$$

$$s_{TR}^3 = \begin{cases} u_R + a_R \sqrt{\frac{\gamma+1}{2\gamma} \frac{p_*}{p_R} + \frac{\gamma-1}{2\gamma}}, & p_* > p_R \\ u_* + a_R \left(\frac{p_*}{p_R} \right)^{(\gamma-1)/2\gamma}, & p_* \leq p_R \end{cases} \quad (27)$$

Here $a_L = \sqrt{\gamma p_L / \varrho_L}$, $a_R = \sqrt{\gamma p_R / \varrho_R}$, and γ denotes the adiabatic constant. Further s_{TL}^1 denotes ‘‘unknown left wave speed’’, s_{TR}^3 ‘‘unknown right wave speed’’. Note, that the system (22) - (27) is the system of 6 equations for 6 unknowns $p_*, u_*, \varrho_{*L}, \varrho_{*R}, s_{TL}^1, s_{TR}^3$.

Solution for the Pressure p_*

The combination of the equations (22), (25) gives the implicit equation for the unknown pressure p_*

$$u_L + F_{1L}(p_*) = u_R + F_{3R}(p_*),$$

with

$$F_{1L}(p) = \begin{cases} -(p - p_L) \left(\frac{2}{p + \frac{\gamma-1}{\gamma+1} p_L} \right)^{\frac{1}{2}}, & p > p_L \\ \frac{2}{\gamma-1} a_L \left[1 - \left(\frac{p}{p_L} \right)^{(\gamma-1)/2\gamma} \right], & p \leq p_L. \end{cases}$$

$$F_{3R}(p) = \begin{cases} (p - p_R) \left(\frac{2}{(\gamma+1) p_R} \right)^{\frac{1}{2}}, & p > p_R, \\ -\frac{2}{\gamma-1} a_R \left[1 - \left(\frac{p}{p_R} \right)^{(\gamma-1)/2\gamma} \right], & p \leq p_R. \end{cases}$$

This is a nonlinear algebraic equation, and one cannot express the analytical solution of this problem in a closed form. The solution p_\star can be found as the root of the function $F(p)$ defined as

$$F(p) = F_{3R}(p) - F_{1L}(p) + u_R - u_L. \quad (28)$$

The analysis of this function can be found in [4]. Here we state, that $F(p)$ is monotone and concave. Also the analytic expression for its derivative is available. For a positive solution for the pressure $F(0) < 0$ is required. This gives the *pressure positivity condition*

$$u_R - u_L < \frac{2}{\gamma-1} (a_L + a_R). \quad (29)$$

The Newton method can be used to find the root of $F(p) = 0$. With the pressure p_\star known, we use the equations (22)-(27) to obtain the whole solution.

Remarks

- Once the pressure p_\star is known, the solution on the left-hand side of the contact discontinuity depends only on the left-hand side initial condition (20). And similarly, with p_\star known, only the right-hand side initial condition (21) is used to compute the solution on the right-hand side of the contact discontinuity.
- The solution in $\Omega_L \cup \Omega_{HTL} \cup \Omega_{\star L}$ (across 1 wave) (solvability in general case)
The solution components in $\Omega_L \cup \Omega_{HTL} \cup \Omega_{\star L}$ region must satisfy the system of equations (22)-(24). It is a system of three equations for four unknowns ($Q_{\star L}$, p_\star , u_\star , s_{TL}^1). We have to add another equation in order to get the uniquely solvable system in $\Omega_L \cup \Omega_{HTL} \cup \Omega_{\star L}$. This is the key problem for the outlet boundary condition.
- The equation (22) can be written as the *equation for pressure*, see [3]

$$p_\star = E_1(u_\star), \quad (30)$$

$$E_1(u) = \begin{cases} \frac{2p_L + \frac{\gamma+1}{2} \rho_L (u_L - u)^2 + (u_L - u) \sqrt{4\rho_L \gamma p_L + \rho_L^2 \left(\frac{\gamma+1}{2} \right)^2 (u_L - u)^2}}{2}, & u < u_L, \\ p_L \left(\frac{-u + u_L + \frac{2}{\gamma-1} a_L}{\frac{2}{\gamma-1} a_L} \right)^{\frac{2\gamma}{\gamma-1}}, & u_L \leq u < u_L + \frac{2}{\gamma-1} a_L. \end{cases}$$

In our work we use the analysis of this problem also for the solution of the initial-boundary value at the boundary faces.

5 Boundary Condition by Preference of Pressure

Using this boundary condition, we try to prescribe given static pressure at the face. This boundary condition corresponds to the real-world problem, when we deal with the

experimentally obtained pressure distribution at the boundary. The conservation laws must be satisfied in close vicinity to the boundary face. We use the analysis of the incomplete Riemann problem to construct the values for the density and the pressure at each boundary face. The following notation is used (some values are used only for an INLET case)

ρ_B	static density at the boundary (unknown)
p_B	static pressure at the boundary (unknown)
\mathbf{v}_B	velocity vector at the boundary (in global coordinates) (unknown)
u_B	normal component of velocity at the boundary (local coordinates) (unknown)
$\mathbf{n} = (n_1, n_2, n_3)$	unit outer normal to face
ρ_L	static density near the wall, time 0
p_L	static pressure near the wall, time 0
\mathbf{v}_L	velocity vector, state near the wall at time 0
u_L	normal component of velocity, state near the wall at time 0
	$u_L = \mathbf{v}_L \cdot \mathbf{n}$
p_{GIVEN}	given value for the pressure (=desired pressure at the face)
ρ_{GIVEN}	given value for the density (=desired INLET density at the face)
$\mathbf{d} = (d_1, d_2, d_3)$	given INLET velocity direction

At the vicinity of the boundary we solve the modified Riemann problem for the split Euler equations (19), introduced in Section 4, with the left-hand side initial condition (20) and the **complementary conditions** (prescribed pressure).

$$p_\star = p_{GIVEN}, \quad (31)$$

$$p_R = p_\star, \quad (32)$$

Here p_\star denotes the pressure in $\Omega_{\star L} \cup \Omega_{\star R}$ part of the solution of the Riemann problem for the split Euler equations, shown in Section 4. This way we have prescribed the desired pressure value whenever it is possible (see the general form of the solution in Section 4). Now it is possible to use (22),(23),(24) Further we must discuss all the possibilities of the left (shock, rarefaction) and the middle (discontinuity) wave in the solution, which is shown in figure 3. In the case of **outlet** ($u_\star \geq 0$), the transformation of the velocity into the global coordinates is

$$\mathbf{v}_B = \mathbf{n}(u_B - u_L) + \mathbf{v}_L.$$

Here u_B denotes the computed velocity in the normal direction. In the case of an **inlet** ($u_\star < 0$) we must **prescribe another conditions** in order to obtain a uniquely solvable system. Here we may choose (for example) arbitrary density ρ_{GIVEN} and the direction of the velocity \mathbf{d} .

$$\rho_{\star R} = \rho_{GIVEN}, \quad \mathbf{v}_B = \mathbf{d}|\mathbf{v}|, \quad \text{with } \mathbf{v}_B \cdot \mathbf{n} = u_\star \quad (33)$$

Then it is

$$p_B = p_{GIVEN}, \quad \rho_B = \rho_{GIVEN}, \quad \mathbf{v}_B = \frac{du_\star}{\mathbf{d} \cdot \mathbf{n}}.$$

The analysis of this problem was shown also in [3].

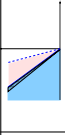
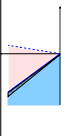

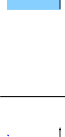

INPUT: $\gamma, \varrho_L, p_L, u_L = v_L \cdot n, p_*, \varrho_{*R}, d$	OUTPUT: ϱ_B, p_B, v_B
$p_* \leq p_L$	$\varrho_L = \sqrt{\gamma \frac{p_*}{p_L}}, \quad s_{HL} = u_L - \varrho_L$ $u_* = u_L + \frac{2}{\gamma-1} \varrho_L \left(1 - \left(\frac{p_*}{p_L} \right)^{\frac{\gamma-1}{2\gamma}} \right)$ $s_{TL} = u_* - \varrho_L \left(\frac{p_*}{p_L} \right)^{\frac{\gamma-1}{2\gamma}}$ $\varrho_{*L} = \varrho_L \left(\frac{p_*}{p_L} \right)^{1/\gamma}$
$p_* > p_L$	$s_1 = u_L - \sqrt{\frac{p_L}{\varrho_L} \sqrt{\frac{\gamma+1}{2\gamma} \frac{p_*}{p_L} + \frac{\gamma-1}{2\gamma}}}$ $u_* = u_L - (p_* - p_L) \left(\frac{\gamma+1}{2\gamma} \frac{p_*}{p_L} + \frac{\gamma-1}{2\gamma} \frac{p_L}{p_*} \right)^{\frac{1}{2}}$ $\varrho_{*L} = \varrho_L \frac{p_L}{p_*} \frac{\gamma+1}{\gamma-1}$
$s_{TL} < 0$	<p>$u_* < 0$</p>  <p>$p_B = p_*$ $u_B = u_*$ $\varrho_B = \varrho_{*R}$ $v_B = \frac{d u_*}{d n}$</p>
$s_{TL} < 0$	<p>$u_* \geq 0$</p>  <p>$p_B = p_*$ $u_B = u_*$ $\varrho_B = \varrho_{*L}$ $v_B = n(u_* - u_L) + v_L$</p>
$s_{TL} \geq 0$	<p>$u_* \geq 0$</p>  <p>$u_B = \frac{2}{\gamma-1} \left[u_L + \frac{\gamma-1}{\gamma} u_* \right]$ $p_B = p_L \left[\frac{2}{\gamma+1} + \frac{\gamma-1}{\gamma+1} \frac{u_L}{u_*} \right]^{\frac{2\gamma}{\gamma-1}}$ $\varrho_B = \varrho_L \left[\frac{2}{\gamma+1} + \frac{\gamma-1}{\gamma+1} \frac{u_L}{u_*} \right]^{\frac{2}{\gamma-1}}$ $v_B = n(\varrho_B - \varrho_L) + v_L$</p>
$s_{TL} \geq 0$	<p>$u_* \geq 0$</p>  <p>$p_B = p_L$ $u_B = u_L$ $\varrho_B = \varrho_L$ $v_B = n(u_* - u_L) + v_L$</p>
$s_1 > 0$	<p>$u_* \geq 0$</p>  <p>$p_B = p_L$ $u_B = u_L$ $\varrho_B = \varrho_L$ $v_B = v_L$</p>

Fig. 3. Algorithm for the solution of the problem (19),(20),(31),(32),(33) at the half line $S_B = \{(0, t); t > 0\}$. The value of the pressure p_* is prescribed. Possible situations are illustrated by the pictures showing $\Omega_L \cup \Omega_{HTL} \cup \Omega_{*L}$ region. The sought boundary state located at the time axis, marked red.

6 Boundary Condition by Preference of Velocity

Here we show the boundary condition preferring the prescribed given velocity at the face. The conservation laws must be satisfied in close vicinity to the boundary face. Therefore we use the analysis of the incomplete Riemann problem to construct the values for the density and the velocity at each boundary face. The following notation is used (some values are used only for an INLET case)

ϱ_B	static density at the boundary (unknown)
p_B	static pressure at the boundary (unknown)
v_B	velocity vector at the boundary (in global coordinates) (unknown)
u_B	normal component of velocity at the boundary (local coordinates) (unknown)
$n = (n_1, n_2, n_3)$	unit outer normal to face
ϱ_L	static density near the wall, time 0
p_L	static pressure near the wall, time 0
v_L	velocity vector, state near the wall at time 0
u_L	normal component of velocity, state near the wall at time 0
$u_L = v_L \cdot n$	
v_{GIVEN}	given velocity vector (=desired value at the face)
u_{GIVEN}	given value for the normal vcomponent of velocity (=desired normal velocity at the face)
$u_{GIVEN} = v_{GIVEN} \cdot n$	
ϱ_{GIVEN}	given value for the density (=desired INLET density at the face)

At the vicinity of the boundary we solve the modified Riemann problem for the split Euler equations (19), introduced in Section 4, with the left-hand side initial condition (20) and the **complementary conditions** (prescribed normal component of velocity).

$$u_* = u_{GIVEN}, \quad (34)$$

$$u_R = u_*, \quad (35)$$

Here u_* denotes the normal component of velocity in $\Omega_{*L} \cup \Omega_{*R}$ part of the solution of the Riemann problem for the split Euler equations, shown in Section 4. This way we have prescribed the desired normal component of velocity whenever it is possible (see the general form of the solution in Section 4). Now it is possible to use (30),(23),(24). Further we must discuss all the possibilities of the left (shock, rarefaction) and the middle (discontinuity) wave in the solution, which is shown in figure 4. The tangential velocities are conserved (same as “left” values) in the case of **outlet** ($u_* \geq 0$), and the velocity vector in the global coordinates is

$$v_B = n(u_B - u_L) + v_L.$$

Here u_B denotes the computed velocity in the normal direction. In the case of an **inlet** ($u_* < 0$) we must **prescribe another conditions** in order to obtain a uniquely solvable system. Here we may choose (for example) arbitrary density ϱ_{GIVEN} and the whole vector of velocity

$$\varrho_{*R} = \varrho_{GIVEN}, \quad v_R = v_{GIVEN}. \quad (36)$$

For example, it is possible to choose the density ϱ_{*R} using the given entropy index $\frac{p_o}{\varrho_o^\gamma}$ (p_o, ϱ_o are some reference values for the pressure and the density)

$$\varrho_{*R} = p_*^{1/\gamma} / \left(\frac{p_o}{\varrho_o^\gamma} \right)^{1/\gamma} = \varrho_o \left(\frac{p_*}{p_o} \right)^{1/\gamma}$$

Another possibility is to conserve (choose) the total temperature θ_0 for the inlet case. Then, using thermodynamic relations (energy equation for a perfect gas), it is

$$\varrho_{\star R} = \frac{p_{\star}}{R\theta_0 \left(1 - \frac{\gamma-1}{2} \frac{|\mathbf{v}_{\text{GIVEN}}|^2}{\gamma R \theta_0}\right)}. \quad (37)$$

Let $\theta_0 = \theta_{0R} = p_R / (R\varrho_R \left(1 + \frac{\gamma-1}{2} \frac{|\mathbf{v}_R|^2}{\gamma p_R / \varrho_R}\right))$ and $\mathbf{v}_{\text{GIVEN}} = \mathbf{v}_R$. Then, using (37), it is $\varrho_{\star R} = \varrho_R \frac{p_{\star}}{p_R}$.

The algorithm for the construction of the primitive variables $\varrho_B, \mathbf{v}_B, p_B$ at the boundary face is shown in Fig. 4. The complete analysis of this problem is shown in [3].

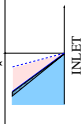
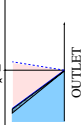

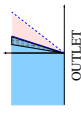
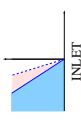
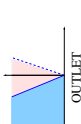
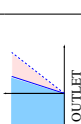
INPUT: $\gamma, \varrho_L, p_L, u_L = \varrho_L \cdot n, u_{\star} = \varrho_R \cdot n, \varrho_{\star R}, \varrho_R$	OUTPUT: $\varrho_B, p_B, \mathbf{v}_B$	
$D = 4\varrho_L \gamma p_L + \varrho_L^2 \left(\frac{\gamma+1}{2} u_L^2 - u_{\star}^2 \right)$ $p_{\star} = \frac{1}{2} \left(2p_L + \frac{\gamma-1}{2} \varrho_L (u_L - u_{\star})^2 + (u_L - u_{\star}) \sqrt{D} \right)$ $s_1 = u_L - \sqrt{\frac{2p_L}{\gamma \varrho_L} \sqrt{\frac{\gamma+1}{2} \frac{p_{\star}}{p_L} + 1}}$ $\varrho_{\star L} = \varrho_L \frac{p_{\star}}{p_L} \frac{1}{\frac{u_L}{u_{\star}} + \frac{1}{\gamma}}$	$a_L = \sqrt{\frac{2p_L}{\gamma \varrho_L}}, \quad s_{HL} = u_L - a_L$ $p_{\star} = p_L \left(\frac{-u_{\star} + u_L + \frac{2}{\gamma-1} a_L}{\frac{2}{\gamma-1} a_L} \right)^{\frac{2\gamma}{\gamma-1}}$ $s_{TL} = u_{\star} - a_L \left(\frac{p_{\star}}{p_L} \right)^{1/\gamma}$ $\varrho_{\star L} = \varrho_L \left(\frac{p_{\star}}{p_L} \right)^{1/\gamma}$	
	$u_{\star} < u_L$	$s_{TL} < 0$  <p>INLET</p> $p_B = p_{\star}$ $u_B = u_{\star}$ $\varrho_B = \varrho_{\star R}$ $\varepsilon_B = \varepsilon_{\star R}$
	$u_{\star} \geq u_L$	$s_{TL} < 0$  <p>OUTLET</p> $p_B = p_{\star}$ $u_B = u_{\star}$ $\varepsilon_B = \varepsilon_{\star L}$ $\mathbf{v}_B = n(u_{\star} - u_L) + \mathbf{v}_L$
	$s_{TL} \geq 0$	$s_{TL} \geq 0$  <p>OUTLET</p> $p_B = p_L \left[\frac{2}{\gamma+1} + \frac{\gamma-1}{\gamma+1} \frac{u_L^2}{a_L^2} \right]^{\frac{2\gamma}{\gamma-1}}$ $u_B = \frac{2}{\gamma+1} \left[u_L + \frac{\gamma-1}{2} u_L \right]$ $\mathbf{v}_B = n(u_B - u_L) + \mathbf{v}_L$ $\varepsilon_B = \varrho_L \left[\frac{2}{\gamma+1} + \frac{\gamma-1}{\gamma+1} \frac{u_L^2}{a_L^2} \right]^{\frac{2}{\gamma-1}}$
$u_{\star} < u_L$	$s_{HL} \geq 0$  <p>OUTLET</p> $p_B = p_L$ $u_B = u_{\star}$ $\varrho_B = \varrho_L$ $\varepsilon_B = \varepsilon_L$	
$u_{\star} \geq u_L$	$s_1 < 0$  <p>INLET</p> $p_B = p_{\star}$ $u_B = u_{\star}$ $\varrho_B = \varrho_R$ $\varepsilon_B = \varepsilon_{\star R}$	
$s_1 \geq 0$	$s_1 \geq 0$  <p>OUTLET</p> $p_B = p_{\star}$ $u_B = u_{\star}$ $\varepsilon_B = \varepsilon_{\star L}$ $\mathbf{v}_B = n(u_{\star} - u_L) + \mathbf{v}_L$	
$s_1 \geq 0$	$s_1 \geq 0$  <p>OUTLET</p> $p_B = p_L$ $u_B = u_{\star}$ $\varrho_B = \varrho_L$ $\varepsilon_B = \varepsilon_L$	

Fig. 4. Algorithm for the solution of the problem (19),(20),(34),(35),(36) at the half line $S_B = \{(0, t); t > 0\}$. Possible situations are illustrated by the pictures showing the region $\Omega_L \cup \Omega_{HTL} \cup \Omega_{\star L}$ with the sought boundary state located at the time axis.

7 Boundary Condition for the Imermeable Wall

Slip wall (Eulerian, inviscid, symmetric boundary)

Using this boundary condition, we set the normal component velocity at the wall to zero. The conservation laws must be satisfied in close vicinity to the boundary face. We use the analysis of the incomplete Riemann problem to construct the values for the density and the pressure at each boundary face. The following notation is used

- ϱ_w static density at the wall
- p_w static pressure at the wall
- \mathbf{v}_w velocity vector at the wall (in global coordinates)
- $\mathbf{n} = (n_1, n_2, n_3)$ unit outer normal to face
- ϱ_L static density near the wall, time 0
- p_L static pressure near the wall, time 0
- \mathbf{v}_L velocity vector, state near the wall at time 0
- u_L normal component of velocity, state near the wall at time 0
- $u_L = \mathbf{v}_L \cdot \mathbf{n}$

At the vicinity of the boundary we solve the following problem (modified Riemann problem for the split Euler equations), with the left-hand side initial condition and the complementary condition (zero normal velocity at the boundary)

$$u_{\star} = 0. \quad (38)$$

Using the analysis shown above (Section 4), the solution of the system (19),(20),(38) lead us to the equations (30), (23). There are two possibilities.

- $u_L > 0$ (1-shock wave)

$$p_w = p_{\star} = \frac{2p_L + \frac{\gamma+1}{2} \varrho_L u_L^2 + u_L \sqrt{4\varrho_L \gamma p_L + \varrho_L^2 \left(\frac{\gamma+1}{2}\right)^2 u_L^2}}{2},$$

$$\varrho_w = \varrho_L \frac{\frac{\gamma-1}{\gamma+1} \frac{p_L}{p_{\star}} + 1}{\frac{p_L}{p_{\star}} + \frac{\gamma-1}{\gamma+1}}.$$

- $u_L \leq 0$ (1-rarefaction wave)

$$p_w = p_L \left(1 + \frac{\gamma-1}{2} \frac{u_L}{a_L} \right)^{\frac{2\gamma}{\gamma-1}}, \quad \text{with } a_L = \sqrt{\gamma p_L / \varrho_L},$$

$$\varrho_w = \varrho_L \left(1 + \frac{\gamma-1}{2} \frac{u_L}{a_L} \right)^{\frac{2}{\gamma-1}}.$$

The velocity in local coordinates is $(0, v_L, w_L)$. The backward transformation of the computed values back into global coordinates (transformation of the velocity components) gives the sought velocity vector at the boundary

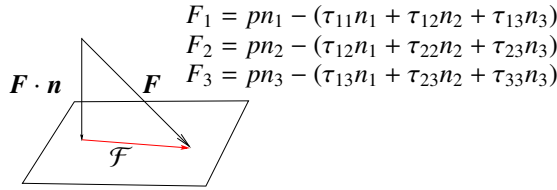
$$\mathbf{v}_w = \mathbf{v}_L - u_L \mathbf{n} = (v_{L1} - u_L n_1, v_{L2} - u_L n_2, v_{L3} - u_L n_3).$$

Remark. It is possible to solve this boundary problem by prescribing the special right-hand side initial condition to the original Riemann problem, described in Section 4., i.e. $\varrho_R = \varrho_L, u_R = -u_L, p_R = p_L$.

Non-slip wall

For the non-slip wall (viscous flow) we set the velocity vector $\mathbf{v}_w = 0$ at the boundary. The turbulent kinetic energy at such non-slip wall is $k = 0$. For the evaluation of the specific dissipation at the boundary ω we use the statements from [1]. Let us use the following notation and relations

θ_w	static temperature at the wall
μ_w	dynamic viscosity at the wall, using Sutherland's law
$\mu_w = \mu_Z \left(\frac{\theta_w}{\theta_Z}\right)^{3/2} \frac{\theta_Z + \theta_S}{\theta_w + \theta_S}$, $\theta_S = 110$, $\theta_Z = 273.15$, $\mu_Z = 1.716 \cdot 10^{-5}$	
k_w	turbulent kinetic energy at the wall, $k_w = 0$
ω_w	turbulent specific dissipation at the wall
$\mathbf{n} = (n_1, n_2, n_3)$	unit outer normal to face
$\mathbf{F} = (F_1, F_2, F_3)$	force (vector) acting on surface



$$\begin{aligned} \tau_{11} &= \frac{2}{3}\mu_w \left(2\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3} \right) & \tau_{12} &= \mu_w \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) \\ \tau_{22} &= \frac{2}{3}\mu_w \left(-\frac{\partial v_1}{\partial x_1} + 2\frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_3} \right) & \tau_{13} &= \mu_w \left(\frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1} \right) \\ \tau_{33} &= \frac{2}{3}\mu_w \left(-\frac{\partial v_1}{\partial x_1} - \frac{\partial v_2}{\partial x_2} + 2\frac{\partial v_3}{\partial x_3} \right) & \tau_{23} &= \mu_w \left(\frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2} \right) \end{aligned}$$

\mathcal{F}	surface shear stress, friction tension (force magnitude in surface direction)
	$\mathcal{F}^2 = F_1^2 + F_2^2 + F_3^2 - (\mathbf{F} \cdot \mathbf{n})^2$
u_τ	friction velocity (velocity scale)
	$u_\tau^2 = \frac{\mathcal{F}}{\rho_w}$

In the real application it is necessary to prescribe the static temperature of the surface θ_w .

The law of wall, [1, pages 13-18]

The law of the wall is empirically-determined relation between the streamwise velocity U and distance from surface y , see [1, page 15]

$$U^+ = \frac{1}{\kappa} \ln(y^+) + C, \quad \text{with} \quad U^+ = \frac{U}{u_\tau}, \quad y^+ = \frac{u_\tau y}{\mu} \quad (39)$$

Measurements indicate $C \approx 5.0$ for smooth surfaces, $\kappa \approx 0.41$ (Karman's constant) for smooth and rough surfaces, y denotes the distance from surface. For the rough surface, with elements of average height k_S , experiments show that the C is a function of k_S ,

$$C \rightarrow 8.5 - \frac{1}{\kappa} \ln k_S^+, \quad \text{where} \quad k_S^+ = \frac{u_\tau \rho_w}{\mu} k_S.$$

Here k_S^+ is dimensionless roughness height. The the law of the wall (39) then yields

$$\frac{U}{u_\tau} = \frac{1}{\kappa} \ln \left(\frac{y}{k_S} \right) + 8.5 \quad (\text{completely rough wall})$$

There is no viscosity in this relation, corresponding with the idea that the "shear stress" is due to pressure drag on the roughness elements. The last relation can be rewritten

as

$$\frac{U}{u_\tau} = \frac{1}{\kappa} \ln \left(\frac{y}{z_S} \right), \quad \text{with} \quad z_S = k_S e^{-8.5\kappa}.$$

Condition for ω , smooth wall

In the case of smooth wall we use the relation

$$\omega_w = 120 \frac{\mu_w}{\rho_w y_S^2},$$

where y_S is the distance of the face from the center of the adjacent element.

Condition for ω , completely rough wall

We simulate the surface roughness by modification of the turbulent dissipation ω at the wall, as described in [1][page 175-177,308].

$$\omega_w = \frac{u_\tau^2 \rho_w}{\mu_w} S_R$$

The coefficient S_R is defined with the use of the roughness height $k_S = z_S e^{8.5\kappa}$

$$S_R = \begin{cases} (50/k_S^+)^2, & k_S^+ \leq 25 \\ 100/k_S^+, & k_S^+ > 25 \\ ([1][page 308] \quad 500/(k_S^+)^{3/2}, & k_S^+ > 25 \end{cases}.$$

Here k_S represents the roughness height. S_R is a continuous function of k_S^+ .

7.1 The Flat Plate Example

Here we show example of the compressible viscous flow along the flat plate. The velocity regime $u = 15 \text{ m s}^{-1}$. The total pressure $p_o = 101325 \text{ Pa}$, total temperature $\theta_o = 273.15 \text{ K}$, and properties $R = 287.04 \text{ J K}^{-1} \text{ mol}^{-1}$, $\gamma = 1.4$, gas flows from the left to the right side. Initial condition for the computation is given by isentropic approximation (and the use of energy equation for a perfect gas)

$$p = p_o \left(1 - \frac{\gamma - 1}{2} u^2 / (\gamma R \theta_o) \right)^{\frac{\gamma}{\gamma - 1}} \approx 101179.69 \text{ Pa},$$

$$\rho = \rho_o \left(1 - \frac{\gamma - 1}{2} u^2 / (\gamma R \theta_o) \right)^{\frac{1}{\gamma - 1}} \approx 1.291 \text{ kg m}^{-3},$$

The initial conditions for the free stream turbulent kinetic energy k and the specific turbulent dissipation ω are given by the turbulent intensity $I = 0.1$ and $\mu_T / \mu = 0.01$:

$$k = \frac{3}{2} v^2 I^2, \quad \omega = \frac{\rho k}{\mu \left(\frac{\mu_T}{\mu} \right)}.$$

($k = 3.375 \text{ m}^2 \text{ s}^{-2}$, $\omega = 2.53995e + 07 \text{ s}^{-1}$, $\mu = 1.716e - 05 \text{ kg m}^{-1} \text{ s}^{-1}$). The computation was made for the simulation of the rough wall (bottom channel wall) with the roughness parameter $z_S = 0.0002$, see figures 5 and 6, the formula for ω at wall was chosen accordingly to [1][page 177].

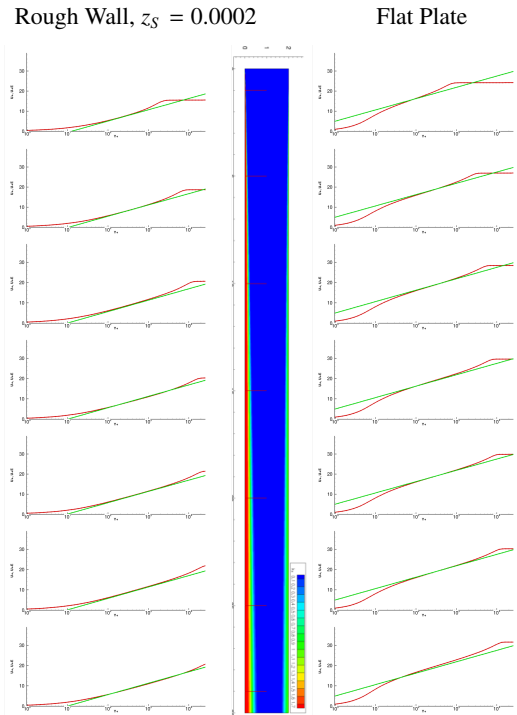


Fig. 5. Computational simulation, the flow along the flat plate and along the rough wall ($z_S = 0.0002$) simulation, regime 15 m s^{-1} , isolines of k turbulent kinetic energy. The $Y^+ - U^+$ graph (log scale) at chosen line cuts (marked by the lines in the central picture). The dotted line shows U^+ given by (39), full line shows the computed results.

7.2 Numerical Tests on Shortened Domains

In order to achieve faster computations it is desired to use smaller computation areas. In such case, the boundary conditions must be chosen appropriately. Here we present numerical experiments with the boundary conditions on smaller domains. At first we assume the compressible viscous flow in the long channel (x-coordinate from -13 to 4), with only small area of interest (x-coordinate from -1 to 2). The velocity regime $u = 15 \text{ m s}^{-1}$. The total pressure $p_o = 101325 \text{ Pa}$, total temperature $\theta_o = 273.15 \text{ K}$, and the gas constants set to $R = 287.04 \text{ J K}^{-1} \text{ mol}^{-1}$, $\gamma = 1.4$, gas flows from the left to the right side. Initial condition for the computation is given by isentropic approximation (and the use of energy equation for a perfect gas). The initial conditions for the free stream turbulent kinetic energy k and the specific turbulent dissipation ω are given by the turbulent intensity $I = 0.1$ and $\mu_T/\mu = 0.01$, see also section 7.1. The results are depicted in figure 7.

The computed results were used in another series of computations on shortened domain (with y-coordinate -1 to 2), in order to test various boundary conditions. The aim was to test various boundary and initial conditions in order to match previously computed data on the original (longer) channel. Here we present the results using the boundary conditions given by the preference of pressure at the outlet, and with the preference of total quantities and the direction of velocity at the inlet. The input values for these boundary conditions were given from the previous computation on larger domain (different values at each boundary face). Results are shown in figures 8 - 10.

Further we show the simulation of emission of another gas specie into the area. We choose the additional gas with

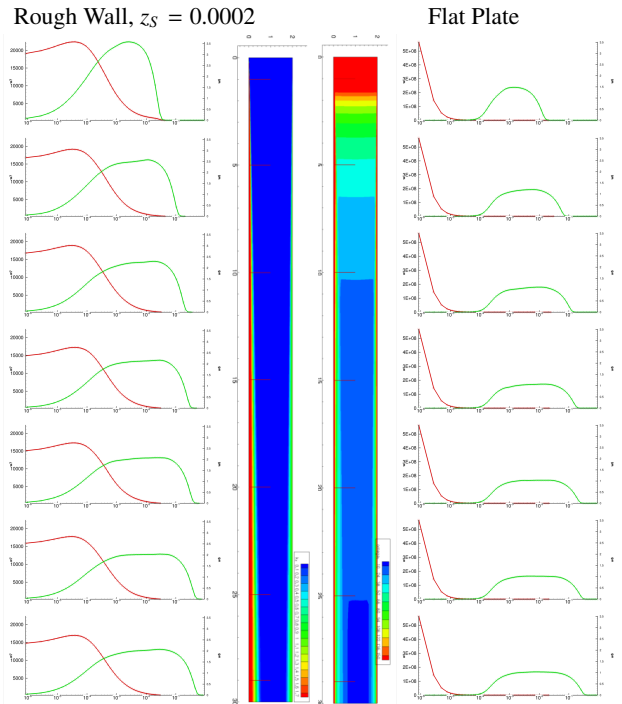


Fig. 6. Computational simulation, the flow along the flat plate and along the rough wall ($z_S = 0.0002$) simulation, regime 15 m s^{-1} , isolines of the turbulent kinetic energy k and dissipation ω . The wall distance - k (green) and ω (red) graphs at the chosen line cuts (marked by the lines in the central picture).

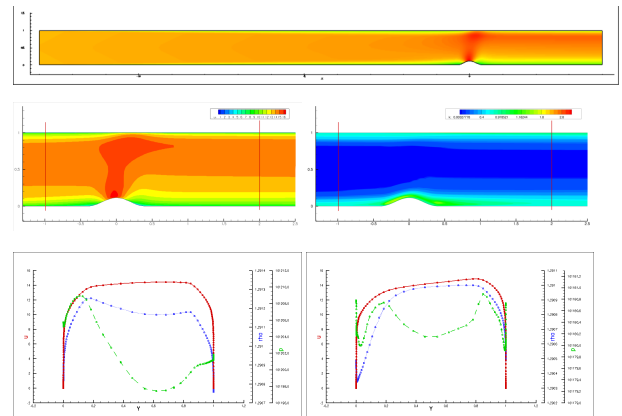


Fig. 7. The flow inside the simple channel with bump, regime 15 m s^{-1} , isolines of u velocity component and k turbulent kinetic energy. The $y - \rho, u, p$ graphs at chosen line cuts (shown red).

the properties $R = 461 \text{ J K}^{-1} \text{ mol}^{-1}$, $c_V = 1450 \text{ J K}^{-1} \text{ mol}^{-1}$, which enters the area. This emission is realized by introducing the fixed source located at the given cell (with cell center coordinates $[0.092, 0.0997, 0.5]$). The mass fraction of additional gas component at this cell was fixed to $Y_1 = 1$, and density was set accordingly to equation of state, using the computed pressure and temperature. Figure 11. shows the propagation of mixture in time.

Conclusion

This paper shows the formulation of the equations describing the mixture of two inert perfect gases in 3D, it is further focused on the boundary conditions and simulation of

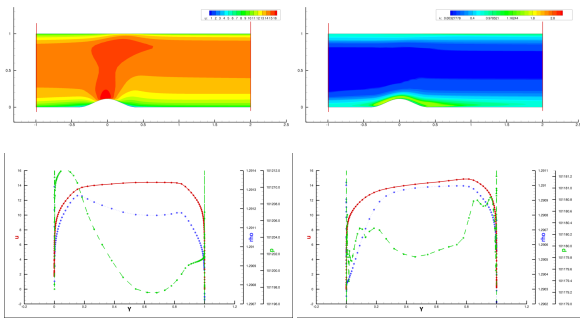


Fig. 8. Computational results on shortened domain. Inlet: fixed “ghost cell” values, outlet: fixed “ghost cell” values.

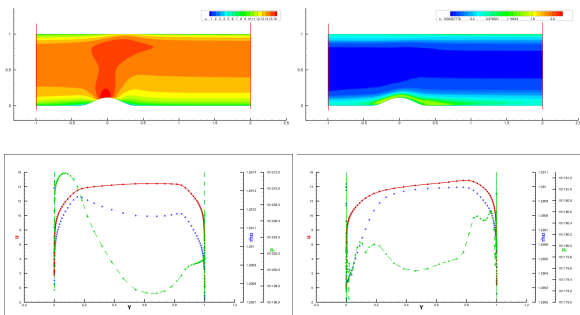


Fig. 9. Computational results on shortened domain. Inlet: fixed “ghost cell” values, outlet: preference of velocity

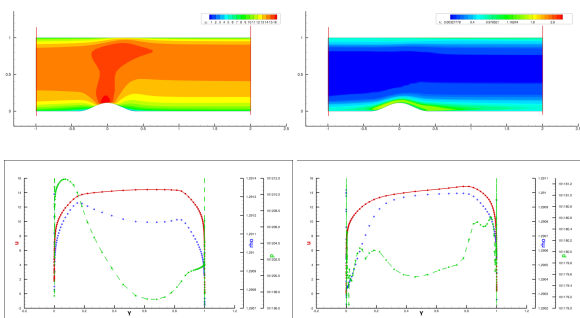


Fig. 10. Computational results on shortened domain. Inlet: preference of total quantities, outlet: preference of pressure.

the wall roughness. 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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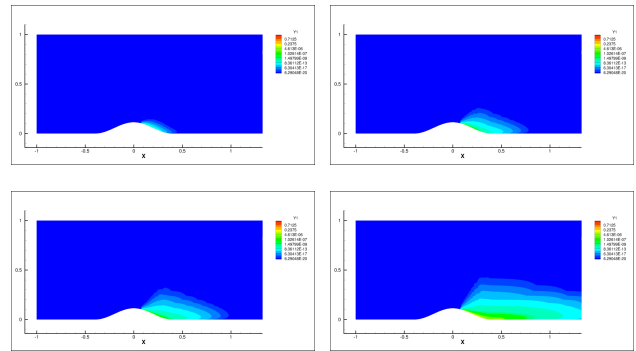


Fig. 11. Computational results on shortened domain. Isolines of 1st specie mass fraction Y_1 in time.

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