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ATMOSPHERIC DISPERSION SIMULATIONS - PASSIVE GAS MIXTURE FLOW

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Abstract: *Here we work with the system of equations describing the non-stationary compressible turbulent multi-component flow in the gravitational field, and we focus on the numerical solution of these equations. The mixture of perfect inert gases is assumed. The RANS equations are discretized with the use of the finite volume method. The exact solution of the modified Riemann problem (original results) is used at the boundary faces. The roughness of the surface is simulated using the alteration of the specific dissipation at the wall. The presented computational results are computed with the own-developed code (C, FORTRAN, multiprocessor, unstructured meshes in general).*

Keywords: Gas Mixture, RANS, Riemann Problem, Software, 3D.

1. Introduction

The physical theory of the compressible fluid motion is based on the principles of conservation laws of mass, momentum, and energy. The mathematical equations describing these fundamental conservation laws form a system of partial differential equations. The aim of this work is to numerically simulate the 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.

$$\frac{\partial \rho Y_1}{\partial t}+\frac{\partial \rho Y_1 v_2}{\partial x_1}+\frac{\partial \rho Y_1 v_2}{\partial x_2}+\frac{\partial \rho Y_1 v_2}{\partial x_3}=\sum_{s=1}^{3}\frac{\partial}{\partial x_s}(\sigma_C \mu_T \frac{\partial Y_1}{\partial x_s})+S_{Y_1} \qquad (1)$$

Here t is time, x_1, x_2, x_3 are the space coordinates, v_1, v_2, v_3 are the velocity components, Y_1 is the mass fraction of the additional gas specie, $\sigma_C \mu_T$ is the diffusion coefficient, and S_{Y_1} denotes the source term. We focus on the numerical solution of these equations.

2. Methods

For the discretization of the system we proceed as described in Kyncl & Pelant (2000). We use either explicit or implicit finite volume method in order to discretize the analytical problem, represented by the system of 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 (and its Jacobians) through the edges/faces of the particular elements. One of the most accurate method (and perhaps the most accurate method) is based on the solution of the so-called Riemann problem for the 2D/3D split Euler equations. The analysis of this problem can be found in many books, i.e. see M. Feistauer, J. Felcman, and I. Straškraba (2003), E. F. Toro (1997). Unfortunately, the exact solution of this problem cannot be expressed in a closed form, and has to be computed by an iterative process (to given accuracy). Therefore this method is also one of the most demanding. Nevertheless, on account of the accuracy of the Riemann solver, we decided to use the analysis of the exact solution also for the discretization of the fluxes through the boundary edges/faces. The right-hand side initial condition, forming the local Riemann problem, is not known at the boundary

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faces. In some cases (far field boundary) it is wise to choose the right-hand side initial condition here as the solution of the local Riemann problem with given far field values, which gives better results than the solution of the linearized Riemann problem. It can be shown, see Kyncl (2011), that the right-hand side initial condition for the local problem can be partially replaced by the suitable complementary condition. In order to prescribe some variable (for example pressure) by chosen value at the boundary, the local modified Riemann problem must have a solution, otherwise the value cannot be used at the boundary. This was the main idea behind the construction of the shown boundary conditions by preference of certain variable. On the contrary to the solution of the initial-value Riemann problem, the solution of the modified boundary problems can be written in a closed form. Therefore it is not computationally expensive to use the constructed boundary conditions in the code. Various original modifications of the Riemann problem (and exact solutions of these modifications) are used at the boundary. In general we prefer the given pressure distribution combined with the given total variables at the inlet.

The own-developed software (C,FORTRAN) is based on the finite volume method with implicit or explicit time discretization, solution is computed on unstructured 3D meshes in general, OpenMPI and MPI parallelizations are used. The large linear systems within the implicit method are solved with the implemented preconditioned GMRES matrix solver. The roughness of the surface is simulated by the adjustment of the specific dissipation at the wall, shown in Wilcox (1998).

3. Examples

In order to simulate the wall roughness we choose the simple channel flow. The air flows over the smooth and rough surface, the channel is 30 m long, regime 15 $m \cdot s^{-1}$. Comparison of the computed values of the normed velocity U^+ (red lines) at the $x_1 = 25m$ (red cut) with the law of the wall, described in Wilcox (1998), shown in Y^+, U^+ graph, figure 1.. Here Y^+ is the normed distance from the wall y.

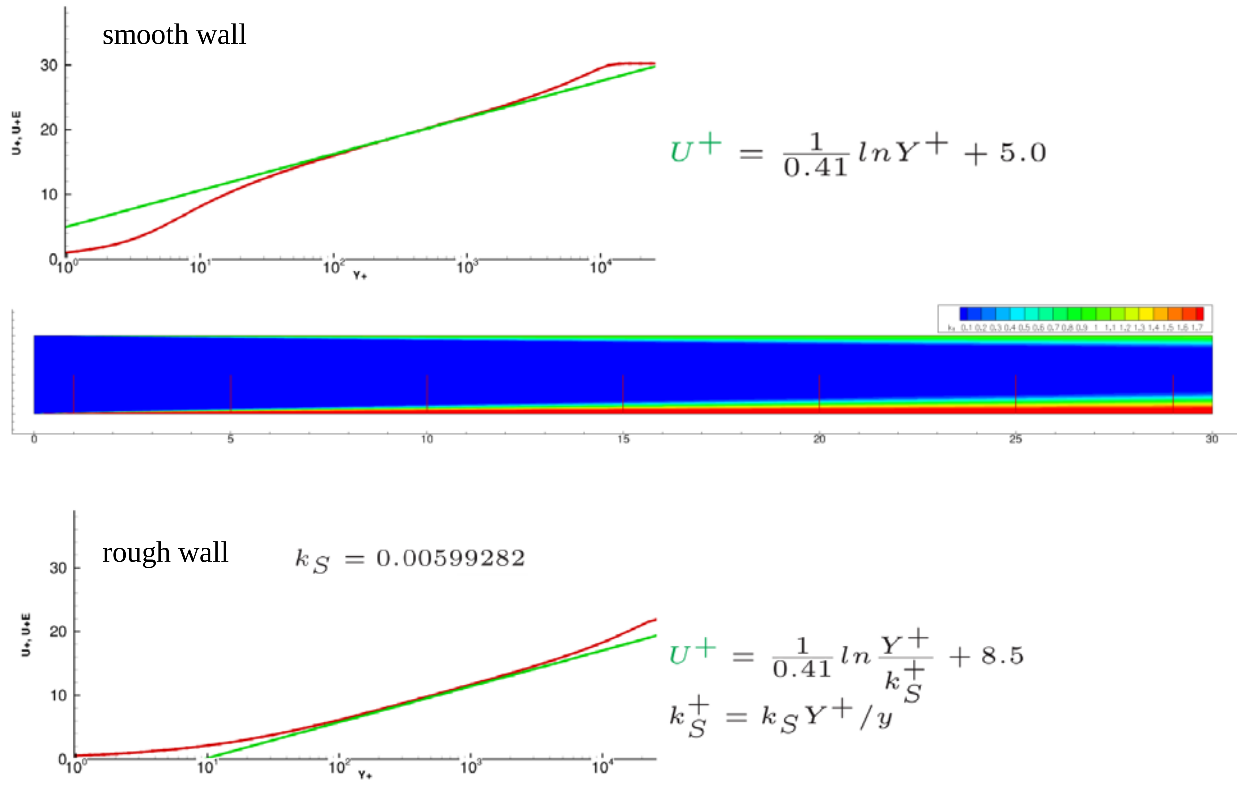

Fig. 1: The wall roughness simulation, channel flow. Isolines of the turbulent kinetic energy and the comparison of the computed data (red line) with the law of the wall (green line).

Further we show the simulation of the gas mixture. The 17 m long channel (with the bump at the bottom wall at the distance 14m) is filled with the air, regime15 $m \cdot s^{-1}$. At the inlet, the boundary condition with the preference of total quantities ($T_0 = 273.15K, p_0 = 101325\,\mathrm{Pa}$) and the direction of velocity (1,0,0) was used, together with the turbulent kinetic energy intensity set to 0.1, turbulent viscosity ratio set to 0.01. Outlet boundary condition by the preference of pressure was used, the pressure value was estimated using the Bernoulli equation for the compressible flow (isentropic relations) for the given regime 15 $m \cdot s^{-1}$. Figure 2. shows the computed distribution of the velocity and the turbulent kinetic energy in the channel, and also in the selected section of the further interest. The computed data from this computation were used for the initial and boundary conditions (the total values conservation at the inlet, pressure preference at the outlet) for the next simulation of the gas mixture propagation. Here the computational area was restricted to the channel section (by x coordinate) from -1 to 2.

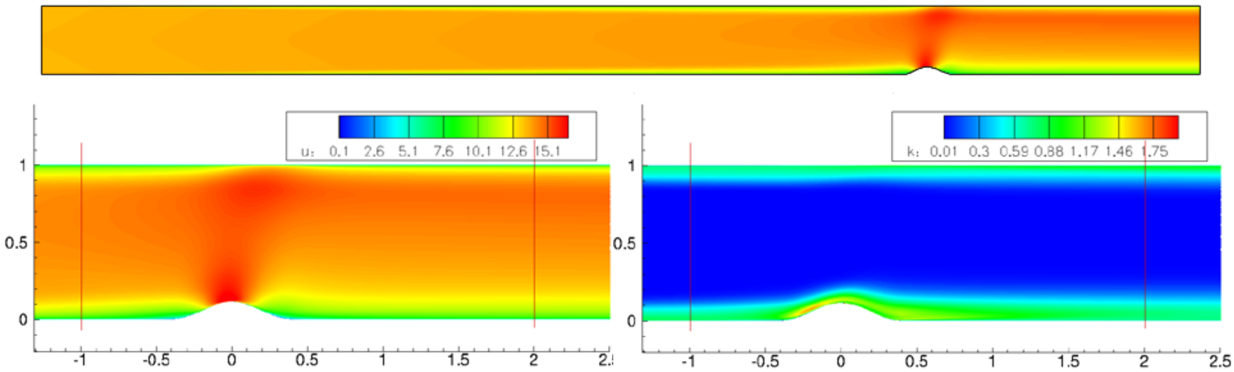

Fig. 2: Channel flow simulation, isolines of the velocity and the specific turbulent kinetic energy.

The additional gas specie enters the area through the boundary condition, fixed source, or with the use of initial condition. The picture sequences in figure 3. demonstrate the propagation of the additional gas specie into the area. Here we tested the various types of the possible pollution source. The computations for the fixed source are visually comparable to the experimentally obtained data.

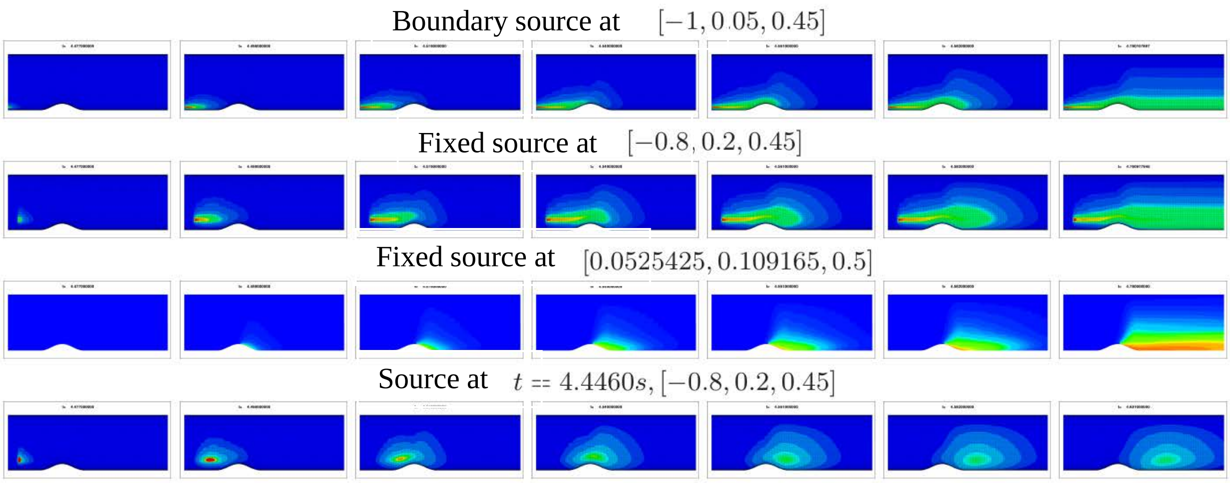

Fig.3: Propagation of the additional gas specie in time, isolines of the mass fraction Y_1.

The figure 4. shows the simplified simulation of the gas mixture flow over the simple terrain. Surface data were given by a set of point coordinates (left picture). Then the surface mesh was constructed and volumes created using own software. Computation run with the regime velocity 4 $m \cdot s^{-1}$, and fixed emission source located at the chosen point. The aim of this computation was to achieve relatively quickly some estimate of the gas dispersion in the case of some possibly dangerous pollution.

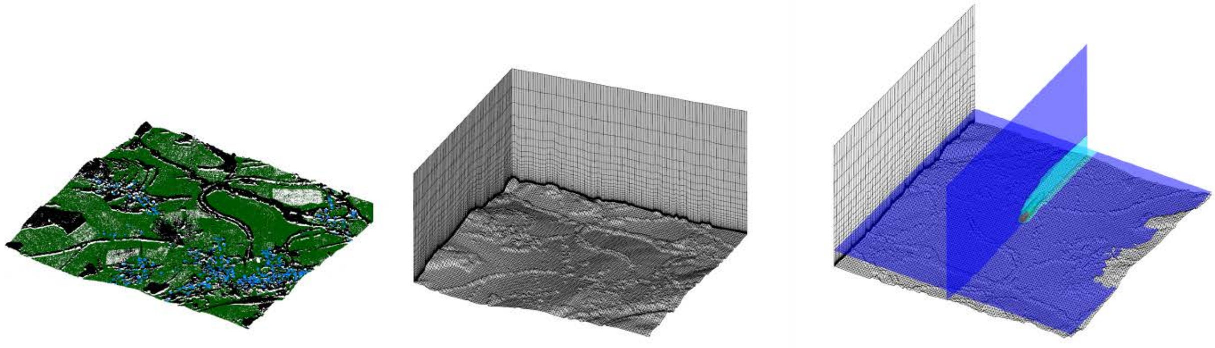

Fig.4: The gas specie dispersion over simple terrain.

4. Conclusions (style - EM 2016 Main chapter)

This paper shows the numerical simulation of 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 and its solution was used at the boundaries. Elementary examples show good coincidence with the experimentally obtained results. The desired intention was to use the modified software for the quick estimation of the gaseous pollution of the air, which 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 set of concentric circles, which is being used now days. Further comparisons with the experimental data (from the wind tunnel) are still in the process.

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