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MATHEMATICAL MODELLING AND NUMERICAL SIMULATION OF POLLUTION TRANSPORT IN THE ATMOSPHERIC BOUNDARY LAYER

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Abstract. Air pollution is one the serious problems in almost all countries, especially those with high population density and large industrial centers. We create a mathematical model based on stationary Navier-Stokes equations for media flow and diffusion-convection equation describing pollution transport, and solve the model using finite element methods (FEMs). The FEMs allows us to use different terrain shapes and examine the terrain influence. An essential part of the work is numerical analysis, which examines the properties of algorithms with respect to numerical parameters, and analyzes selected cases of media flow in the atmospheric boundary layer in the case of instant, steady or periodically interrupted sources of pollution. The most significant results are obtained in direct application to real problems like the transport of pollution caused by a stack with time dependent intensity or the model of an ecological accident.

Key words. pollution transport, diffusion-convection equation, Navier-Stokes equation, finite element method, method of characteristics

AMS subject classifications. 76D05, 76M10, 65M25, 65N30

1. Introduction. We create a 2D model of pollution transport on a polygonal domain Ω which represents a vertical cut through landscape. We consider the case of stationary Navier-Stokes flow and diffusion-convection equation for one type of pollutant. We solve the following system of equations on $(0,T)\times\Omega$:

$$
\begin{aligned}
\frac{\partial c(t,x)}{\partial t} + \vec{v}(x)\,\mathrm{grad}\,c(t,x) &= D\triangle c(t,x) + f(t,x)\\
\vec{v}(x)\nabla\vec{v}(x) - \nu\triangle\vec{v}(x) + \mathrm{grad}\,p(x) &= \vec{g}(x)\\
\mathrm{div}\,\vec{v}(x) &= 0\\
c(0,x) &= c_0(x) \quad x\in\Omega\\
\frac{\partial c}{\partial\vec{n}}\Big|_{terr} = 0 \quad c|_{\partial\Omega} &= c_\Gamma(x)\\
\vec{v}|_{\partial\Omega} &= \vec{v}_\Gamma
\end{aligned}
$$

where $\Omega\subset\mathbb{R}^2$ is a bounded domain derived from a rectangle by substitution of the bottom edge by a piecewise linear line representing the terrain, $c(t,x)$ is the concentration of pollutant, $\vec{v}(x)$ is the velocity, c_0 is the initial condition for concentration, $\frac{\partial c}{\partial\vec{n}}|_{terr}=0$, c_Γ, $\vec{v}_\Gamma$ are boundary conditions for concentration and velocity, where $\vec{n}$ is the unit outer normal and $terr$ denotes the terrain. Dirichlet conditions were considered for easier implementation; compare with [9]. More accurate from physical point

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of view would be Neumann conditions on the outlet for both velocity and concentration $\frac{\partial c}{\partial \vec{n}}|_{out}=0$, $\frac{\partial \vec{v}}{\partial \vec{n}}|_{out}=0$. The term $f(t,x)$ represents the pollution source and $\vec{g}(x)$ is the external force.

If we assume that the pollutant particles have low momentum and low concentration, and thus don't influence airflow retroactively, we can first solve the Navier-Stokes problem and then the diffusion-convection problem with given velocity field $\vec{v}(x)$.

2. Weak formulation of Navier-Stokes problem. Let $V=(\mathring{W}_2^{(1)}(\Omega))^2$, $X=(W_2^{(1)}(\Omega))^2$, $H=\{q\in L^2(\Omega):\int_\Omega q\,dx=0\}$, $\vec{w}\in X$: $\vec{w}\,|_{\partial\Omega}=\vec{v}_\Gamma$ in weak sense, $\int_{\partial\Omega}\vec{w}\vec{n}\,dS=\int_\Omega \operatorname{div}\vec{u}\,dx=0$ for Dirichlet boundary condition. We denote $\vec{u}=\vec{v}-\vec{w}$

$((\vec{w},\vec{s}))=\int_\Omega\sum_{i,j=1}^{2}\frac{\partial w_i}{\partial x_j}\frac{\partial s_i}{\partial x_j}=(\nabla\vec{w},\nabla\vec{s})$, $\quad b(\vec{u},\vec{v},\vec{s})=\frac{1}{2}\int_\Omega\sum_{i,j=1}^{2}(u_j\frac{\partial v_i}{\partial x_j}s_i-u_jv_i\frac{\partial s_i}{\partial x_j})$

We seek $v\in X$ and $p\in H$, such that:

$$((\vec{v},\vec{s}))+b(\vec{v},\vec{v},\vec{s})-(p,\operatorname{div}\vec{s})=(\vec{g},\vec{s})-((\vec{w},\vec{s}))\qquad\forall\vec{s}\in V$$
$$(q,\operatorname{div}\vec{u})=-(q,\operatorname{div}\vec{w})\qquad\forall q\in H$$

Index h denotes finite-dimensional subspaces $V^h\subset V$, $X^h\subset X$, $H^h\subset H$. The mixed formulation in finite-dimensional case stands:

$$((\vec{v}^h,\vec{s}))_h+b_h(\vec{v}^h,\vec{v}^h,\vec{s}^h)-(p^h,\operatorname{div}_h\vec{s})_h=(\vec{g}^h,\vec{s})_h-((\vec{w}^h,\vec{s}))_h$$
$$(q,\operatorname{div}_h\vec{u}^h)_h=-(q,\operatorname{div}_h\vec{w}^h)_h\qquad\forall\vec{s}\in V^h\quad\forall q\in H^h$$

The nonlinear term $b_h(\vec{u}^h,\vec{u}^h,\vec{s}^h)$ must be computed iteratively. Direct application of this approach gives solution with oscillations. A suitable way is to use the upwind scheme for finite element method by [6], which uses the dual triangulation[1].

$$\begin{pmatrix}\mathbf{A}(u^k) & \mathbf{B}\\ \mathbf{B}^T & 0\end{pmatrix}\begin{pmatrix}u^k\\ -p^k\end{pmatrix}=\begin{pmatrix}G\\ H\end{pmatrix}$$

3. Rothe Method and the Method of Characteristics for diffusion-convection equation. We use implicit Rothe method [4] to deal with time derivative $\frac{\partial c}{\partial t}(t,x)=\frac{c(t,x)-c(t-\tau,x)}{\tau}$, where τ is the timestep. For timelevel $k\tau$, $k=0,\dots,T/\tau$ we obtain:

$$c(k\tau,x)-\tau D\triangle c(k\tau,x)+\tau\vec{v}\,\nabla c=\tau f(k\tau,x)+c((k-1)\tau,x)$$

Direct application of this approach leads to the oscillatory scheme with nonsymetric matrix. One possible way to remove these properties is to use the method of characteristics [5]. Let $V=\mathring{W}_2^{(1)}(\Omega)$, $w\in W_2^{(1)}(\Omega)$: $w|_{\partial\Omega}=c_\Gamma(x)$ in weak sense. The main idea of the method is to separate both parts of the process. The convective part is represented by the instant shift of concentration field using mapping $\varphi^k(x)=x-\tau\vec{v}(k\tau,x)$ Making scalar product with a function $v\in V$ we have $\forall v\in\mathring{W}_2^{(1)}(\Omega)$

$$(c^k,v)+\tau D(\nabla(c^k-w),\nabla v)=(\tau f^k+c^{k-1}\circ\varphi^k,v)-\tau D(\nabla w,\nabla v)$$

Restriction to finite-dimensional subspace $V^m\subset V$ and standard Galerkin approximation give a linear system with positive-definite matrix. For $i=1,\dots,m$:

$$\sum_{j=1}^{m}\alpha_j^k[(v_j,v_i)+\tau D(\nabla v_j,\nabla v_i)]=(\tau f^k+c^{k-1}\circ\varphi^k,v_i)-\tau D(\nabla w,\nabla v_i)$$

[1] Uses the barycentric nodes of the original triangulation

4. Triangulation of Domain for Navier-Stokes Problem. When storing general unstructured mesh the required information depends on the type of the problem we solve, consequently on the selected type of finite elements. Also different types of boundary conditions require specific indexing. Although there is some "minimal" sufficient information, obtaining additional data necessary to fill the elements of the matrices for weak solutions is time-expensive.

In our case, we must store following information: for nodes their coordinates, for edges their position - whether they are interior or boundary, indexes of vertices, surrounding edges and triangles, and for triangles their vertices and edges. We must also split the boundary into parts according to the type of the boundary condition.

5. Numerical Solution using the Finite Element Method. The finite element method was selected because it allows an easy solution of the model on domains with different terrain shapes. A simple structured mesh of rectangle type with M nodes in the horizontal direction and N nodes in the vertical direction was used in the simulations. We have chosen linear Lagrange elements for concentration, Cruzeix-Raviart elements for velocity and piecewise constant elements for pressure. Similar elements related to the boundary nodes were used for the approximation of boundary conditions. Very important for the implementation is the fact that both problems lead to rare matrices with only $O(MN)$ nonzero elements.

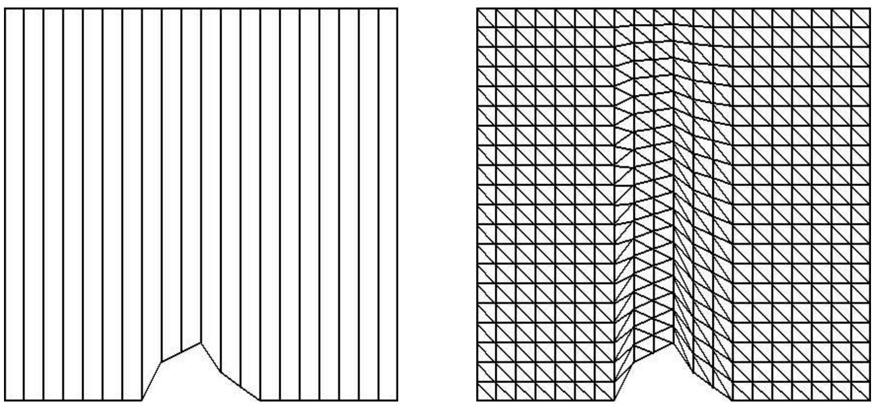

FIG. 5.1. *Structured mesh*

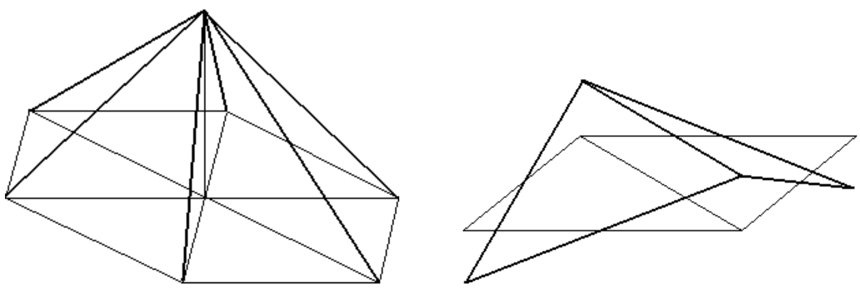

FIG. 5.2. *Lagrange and Cruzeix-Raviart elements*

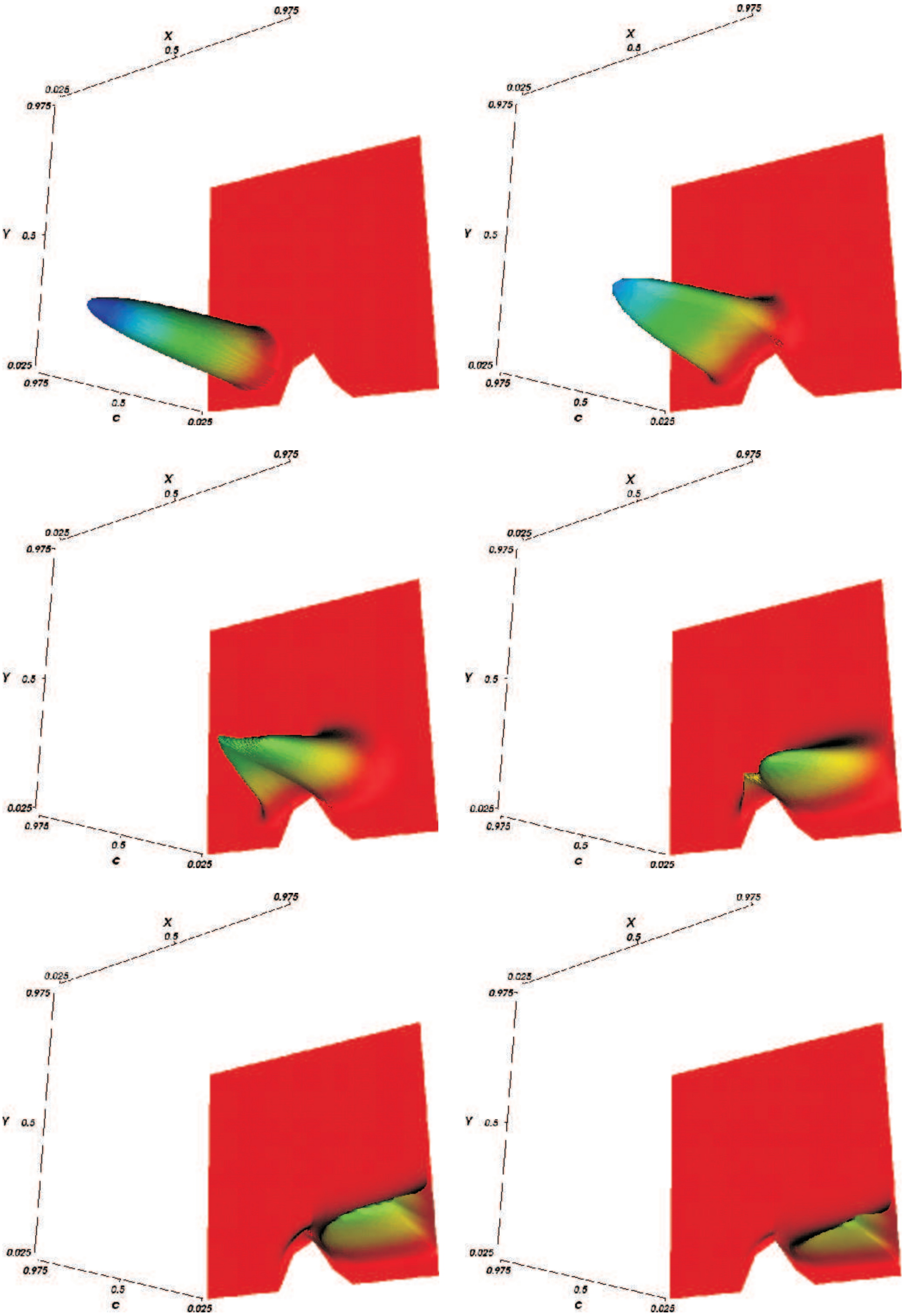

FIG. 5.3. *Accident model - concentration at timesteps 0,100,200,300,400,500; ordered from left to right and from top to bottom*

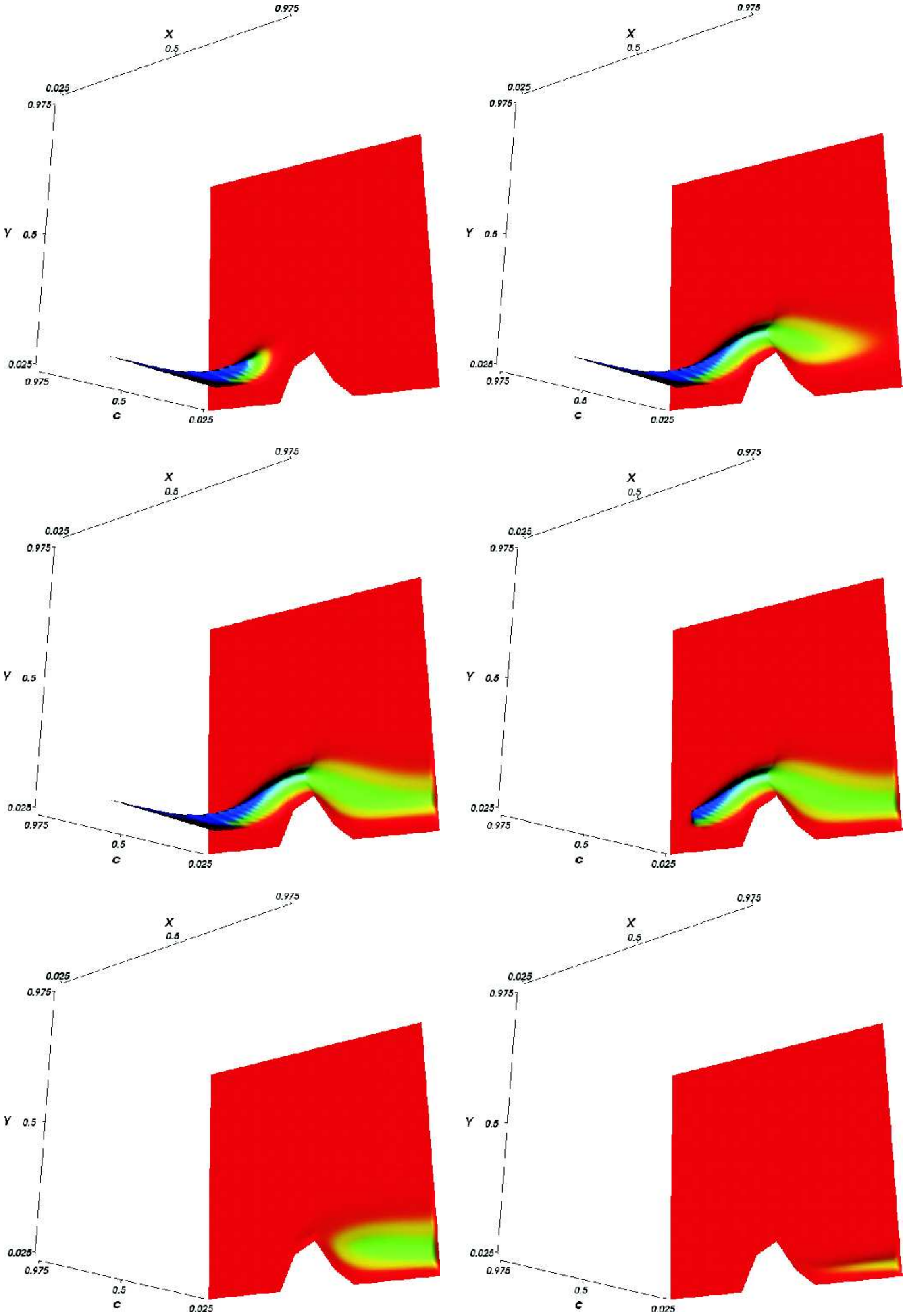

FIG. 5.4. *Steady source model - concentration at timesteps 200,600,900,1100,1500,2000; ordered from left to right and from top to bottom*

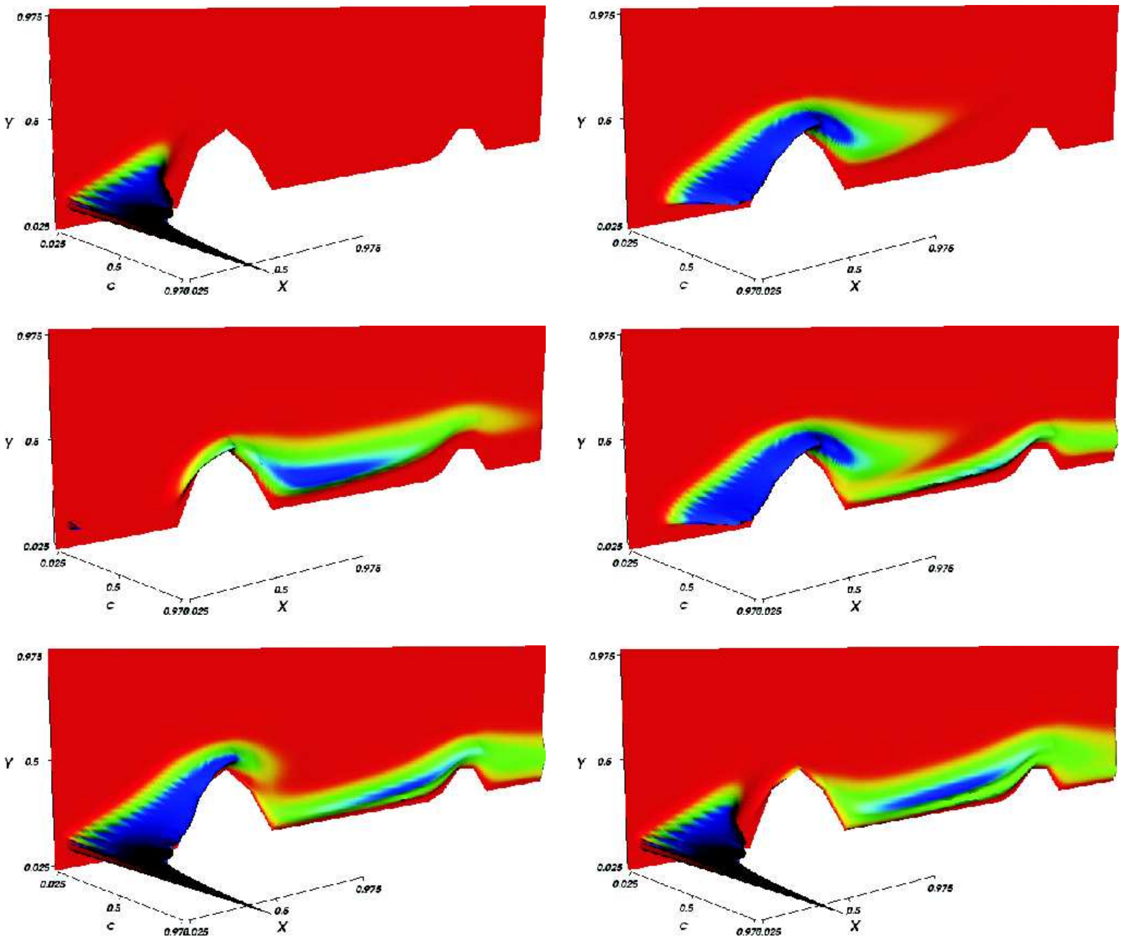

Fig. 5.5. *Pulsing source model - concentration at timesteps 400,1200,2000,3200,4800,6400; ordered from left to right and from top to bottom*

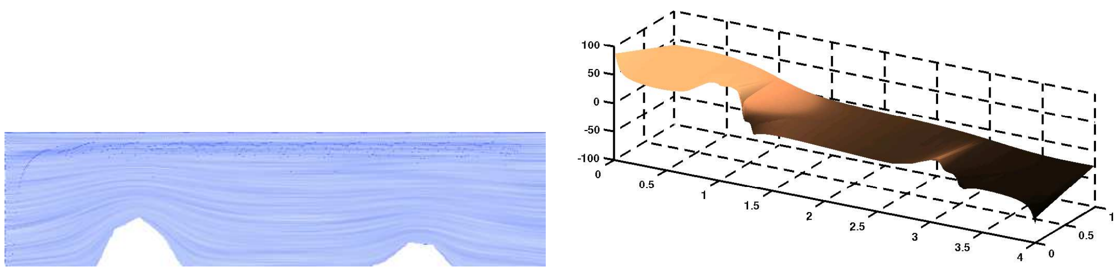

Fig. 5.6. *Velocity and pressure fields - pulsing source*

6. Main results. The following examples show the most important results concerning pollution transport. Stokes flow is considered. Different types of terrain and pollution source are used. The figures show the values of concentration for several timesteps, eventually pressure and velocity fields.

6.1. Example. In t=0 an accident happens and certain amount of pollution is released in the air. The example shows the time development of the pollution cloud and its dissipation due to terrain shape. Concentration levels are shown on Fig.5.3.

6.2. Example. The steady source of pollution. In the middle of the time period the source ceases and then the area becomes clean again. See Fig.5.4.

6.3. Example. The stack, which produces pollution in shifts. Several periods proceed, making significant waves with each shift. See Fig.5.5 and Fig.5.6.

7. Conclusion. We presented a 2D model of pollution transport in the atmospheric boundary layer. The model consists of diffusion-convection equation describing the transport of one passive pollutant in the isothermic flow governed by stationary Navier-Stokes equations. Dirichlet boundary conditions were considered for simplicity. Numerical solution was performed by finite element method. Several examples were tested, using different types of terrain and sources of pollution. An improved model containing Neumann boundary conditions will be finished soon. Main goal of the future work is implementation of a suitable turbulence model and comparison of results with experimental data provided by the Institute of Thermomechanics of Academy of Sciences of the Czech Republic.

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