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MATHEMATICAL AND EXPERIMENTAL MODELLING OF POLLUTANT DISPERSION

MATEMATICKÉ A EXPERIMENTÁLNÍ MODELOVÁNÍ ŠÍŘENÍ POLLUTANTŮ

Abstract

The paper presents mathematical modelling examples of pollutants distribution arising from motor traffic in urban areas. Realized experiment consisted of measurement of nitrogen dioxide and ozone concentration and measurement of the wind speed and direction. As model case the Leger street in Prague was chosen. This is a one-way street with a linear source of pollution. Simple model was created for numerical modelling. The simple model is gradually being solved by start-up the wind, then spread the exhaust gas, the addition of braking force from the car and also the turbulent kinetic energy, which is fanning the substances of moving cars. For mathematical modelling of pollutant dispersion method of finite volume and software Fluent 6.3 was used.

Abstrakt

V článku je prezentován příklad matematického modelování šíření polutantů vzniklých automobilovým provozem v městské zástavbě. Byl proveden experiment, který se sestával z měření koncentrace oxidu dusičitého a ozónu a z měření rychlosti a směru větru. Modelovým případem byla zvolena Legerova ulice v Praze. Jedná se o jednosměrnou ulici s lineárním zdrojem znečištění. Pro numerické modelování byl zatím vytvořen jednoduchý model, ve kterém je postupně řešen rozběh větru, následně šíření výfukových zplodin, přidání brzdné síly od automobilů a také přidána kinetická turbulentní energie, jež představuje rozdmýchávání látek pohybem automobilů. Pro matematické modelování šíření polutantů byl využit software Fluent 6.3. Model byl řešen metodou konečných objemů.

1 INTRODUCTION

Measurement of concentrations of exhaust gases and particles created in the combustion process of the cars units is necessary for populations living in areas with increased traffic because of subsequent possible health complications. This issue is monitored and processed to be proposed as the most effective protection of the population. One way to visualize the trade proposals and determine their efficiency is a numerical modelling. This paper presents one case of the numerical simulation of the pollutants dispersion.

2 MATHEMATICAL MODEL OF TURBULENCE FOR COMPRESSIBLE FLOW

Turbulent k-e model was used for solving of air turbulent flow, which consists of following equations, [3]:

continuity equation

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$$\frac{\partial \rho}{\partial t}+\frac{\partial\left(\rho \bar{u}_j\right)}{\partial x_j}=0\,, \tag{1}$$

momentum equation (Navier-Stokes equation)

$$\frac{\partial\left(\rho \bar{u}_i\right)}{\partial t}+\frac{\partial\left(\rho \bar{u}_i \bar{u}_j\right)}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu_t \frac{\partial \bar{u}_i}{\partial x_j}\right)+\rho\,\delta_{i3} g+\rho\, f_i \tag{2}$$

energy equation

$$\frac{\partial}{\partial t}\left(\rho \bar{E}\right)+\frac{\partial}{\partial x_j}\left(\rho \bar{u}_j \bar{E}\right)=\frac{\partial \bar{p}}{\partial t}+\rho \bar{u}_j f_j+\frac{\partial\left(\tau_{jl} \bar{u}_j\right)}{\partial x_l}+\frac{\partial}{\partial x_j}\left(\lambda_t \frac{\partial \bar{T}}{\partial x_j}\right), \tag{3}$$

species transport equation

$$\frac{\partial}{\partial t}\left(\rho \overline{Y_{i'}}\right)+\frac{\partial}{\partial x_j}\left(\rho \overline{u_j} \overline{Y_{i'}}\right)=-\frac{\partial}{\partial x_j} \cdot J_{i',j}+R_{i'}+S_{i'} \tag{4}$$

evaporisations equation

$$N_{i'}=k_c\left(C_{i',s}-C_{i',\infty}\right), \tag{5}$$

transport equation for kinetic turbulent energy

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial\left(\rho \bar{u}_j k\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k} \cdot \frac{\partial k}{\partial x_j}\right)+\mu_t\left(\frac{\partial \bar{u}_j}{\partial x_l}+\frac{\partial \bar{u}_l}{\partial x_j}\right) \frac{\partial \bar{u}_l}{\partial x_j}-g_j \frac{\mu_t}{\rho \sigma_h} \frac{\partial \rho}{\partial x_j}-\rho \varepsilon \tag{6}$$

dissipation rate equation

$$\frac{\partial(\rho \varepsilon)}{\partial t}+\frac{\partial\left(\rho \bar{u}_j \varepsilon\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon} \cdot \frac{\partial \varepsilon}{\partial x_j}\right)+\rho C_{1\varepsilon}\left(\mu_t\left(\frac{\partial \bar{u}_j}{\partial x_l}+\frac{\partial \bar{u}_l}{\partial x_j}\right) \frac{\partial \bar{u}_l}{\partial x_j}-C_{3\varepsilon} g_j \frac{\mu_t}{\rho \sigma_h} \frac{\partial \rho}{\partial x_j}\right)-\rho C_{2\varepsilon} \frac{\varepsilon^2}{k}\,, \tag{7}$$

where:

i, j = 1, 2, 3
i' – index of specie
$\bar{E}$ – energy $[\mathrm{J \cdot kg^{-1}}]$,
f_i – force $[\mathrm{N}]$,
g – gravity acceleration $[\mathrm{m \cdot s^{-2}}]$,
k – kinetic turbulent energy $[\mathrm{m^2 \cdot s^{-2}}]$,
k_c – mass transfer coefficient $[\mathrm{m \cdot s^{-1}}]$,
$\bar{p}$ – pressure $[\mathrm{Pa}]$,
t – time $[\mathrm{s}]$,
$\bar{u}_i$ – velocity $[\mathrm{m \cdot s^{-1}}]$,
x_i – coordinate $[\mathrm{m}]$,
$C_{i',s}$ – vapour concentration at the droplet surface $[\mathrm{kmol \cdot m^{-3}}]$,
$C_{i',\infty}$ – vapour concentration in the bulk gas $[\mathrm{kmol \cdot m^{-3}}]$,
$J_{i'}$ – diffused flux of species i' $[-]$,

$N_{i'}$ – molar flux of vapor $[\mathrm{kmol \cdot m^{-2} \cdot s^{-1}}]$,

$R_{i'}$ – net rate of production of species i' $[\mathrm{kg \cdot m^{-3} \cdot s^{-1}}]$,

S_i – source of dispersed phase i' defined by the user $[\mathrm{kg \cdot m^{-3} \cdot s^{-1}}]$,

$Y_{i'}$ – mass fraction of species i' $[-]$,

d_{i3} – Kronecker delta $[-]$,

e – dissipation rate $[\mathrm{m^2 \cdot s^{-3}}]$,

l_t – coefficient of turbulent heat conductivity $[\mathrm{W \cdot m^{-1} \cdot K^{-1}}]$,

m_t – turbulent viscosity $[\mathrm{kg \cdot m^{-1} \cdot s^{-1}}]$,

r –density $[\mathrm{kg \cdot m^{-3}}]$,

s_h – Prandtl turbulent number $[-]$,

s_k , s_e , C_{1e} , C_{2e} , C_{3e} , C_d – empirical constants $[-]$,

t_{jl} – tensor of viscous tension $[\mathrm{Pa}]$.

Pollutants dispersion was solved by finite volume method in Fluent 6.3.

3 EXPERIMENT [6]

The Leger street as testing case was chosen to realize the experiment. This street is one of the arteries of the Prague agglomeration, which is a typical street canyon in urban with well-defined line source of pollution, see **Fig. 1**.

Fig. 1 Leger street

Measuring LIDAR system was installed before entering a Leger street. Monitoring was carried out in standard working days in summer and autumn. Field concentrations of nitrogen dioxide in the form of two-dimensional vertical sections of Leger street were repeatedly measured. Vertical incisions were conducted approximately diagonally because of its shape. Obtained data were processed using DIAL method.

Weather has a significant impact on the spread of pollution and the pollutants distribution in the air. Wind speed and direction over the canyon buildings and the temperature at various heights above the ground along the building walls were measured by SODAR. Data on ground-level wind directly in the street canyon were obtained by the anemometer located on the scoring drive air pollution monitoring, see **Fig. 2**.

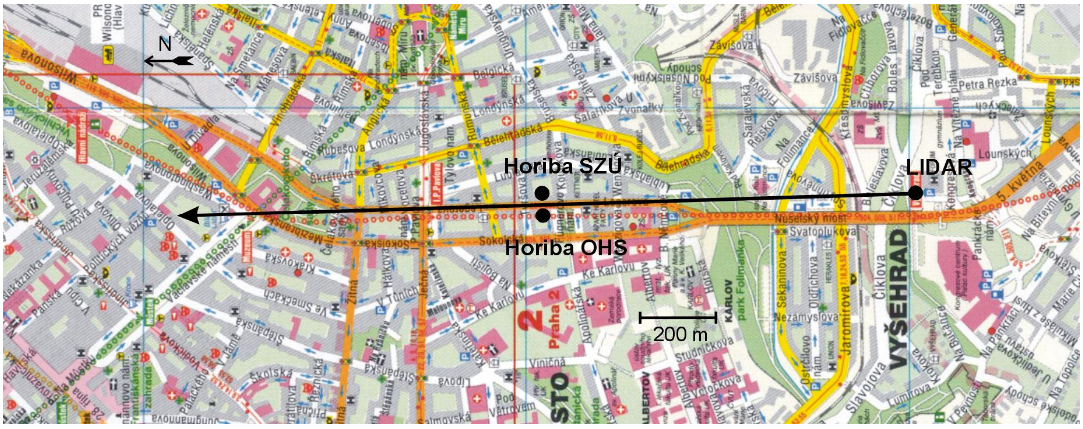

Fig. 2 The direction of vertical sections carried over Leger street, lidar measurement position and the location of mobile stations, air pollution monitoring points (HORIBA) marked on the map

The resulting values of the measured concentrations of nitrogen dioxide NO_2 were graphically presented in time intervals. Nitrogen dioxide is the average value in each monitored hour, see Fig. 3. Concentration values follow the state according to the passing cars number. Nitrogen dioxide concentration is markedly increased during morning rush hour as can be seen in **Fig. 3**.

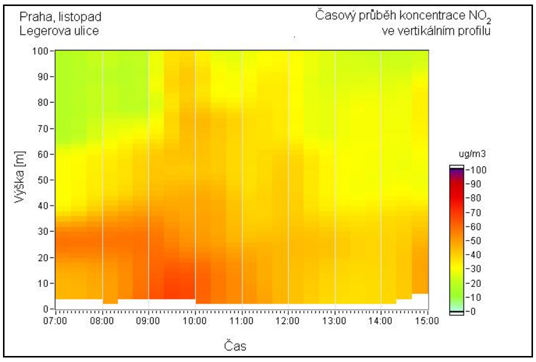

Fig. 3 Time dependence of the vertical distribution of nitrogen dioxide in the atmosphere over Leger street, November.

4 MATHEMATICAL MODEL

Numerical simulation procedure has been tested on a simple geometry consisting of a street canyon (height of buildings to 24 m) and the atmosphere at a height of 200 m. The geometry of the street canyon was created including the volumes of cars and their exhaust, see **Fig. 4**. Firstly computational area and its grid were created in software Gambit. Symmetric boundary conditions were chosen to front and hind geometry (entry and exit of the canyon). Periodic boundary conditions were chosen on the sides of buildings. Roughness of wall buildings boundary condition should was set to 5 mm, which corresponds to the roughness of buildings, [4].

Number of cells was 627 928. The area was exported from Gambit into Fluent 6.3, where the problem by $k-e$ turbulent model was solved.

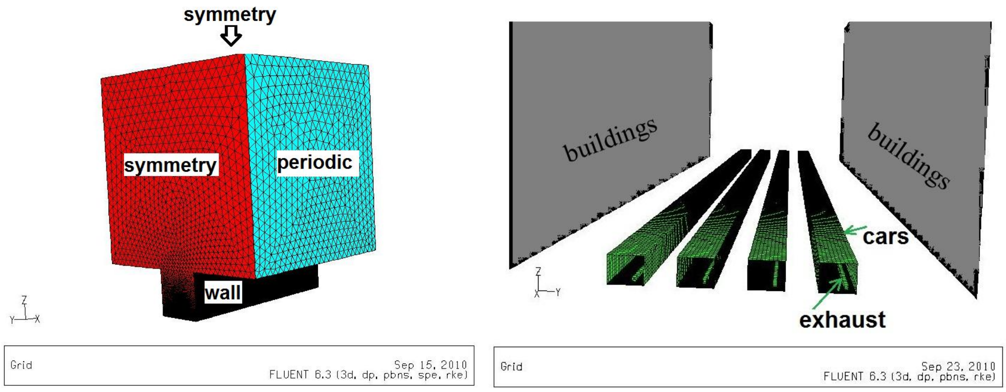

Fig. 4 Computational area

Wind speed and direction were known from measurements. Wind speed was defined by value 4 ms^{-1}. These boundary conditions were commissioned to set up the volume with a height of one cell, see **Fig. 5**. Turbulent kinetic energy was set at 24 $m^2 \cdot s^{-2}$ and dissipation rate was set at 11,5 $m^2 \cdot s^{-3}$ [3].

Properties of nitrogen dioxide [2]:	density	1 $kg.m^{-3}$
	kinematic viscosity	$1{,}72.10^{-5}$ $kg.m^{-1}.s^{-1}$
	mole weight	46,0055 $kg.kmol^{-1}$

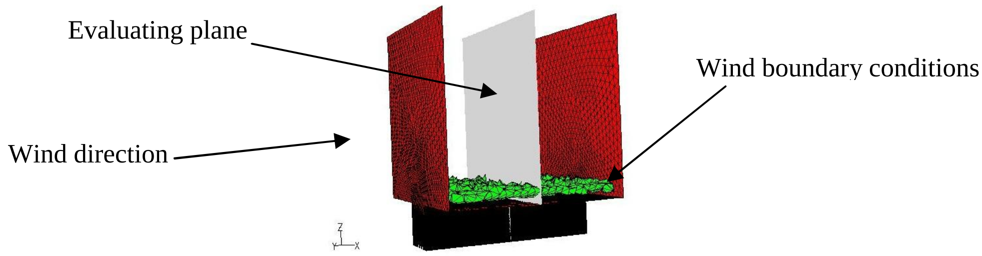

Fig. 5 Computational area, wind enter

5 RESULTS

All shown results are evaluated in the middle plane of computed area, see **Fig. 5**. Wind effect is spread across the field after a few iterative steps, see **Fig. 7**. Intermediate step is shown in **Fig. 6**.

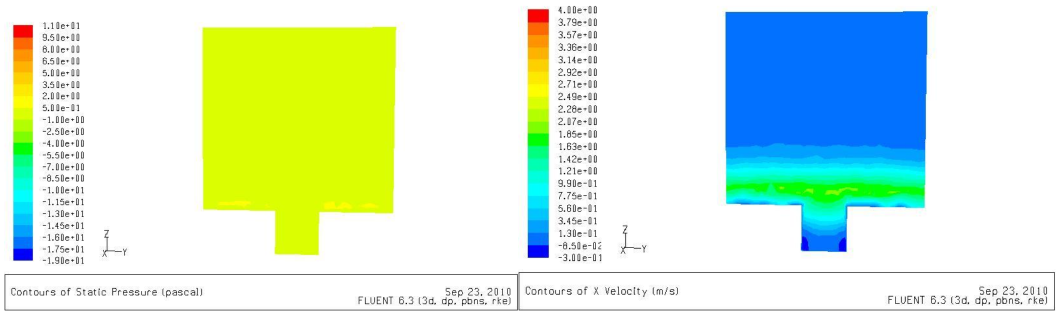

Fig. 6 Start-up wind - pressure and velocity distribution

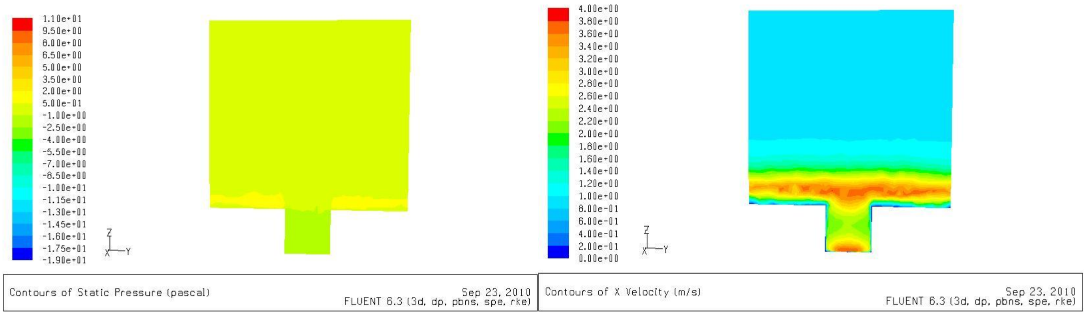

Fig. 7 Steady state wind - pressure and velocity distribution

After steady state wind computation the value of pollutant quantity corresponding to the car density was set using a mixture model. Mass fraction of nitrogen dioxide was 4,03906 .10^{-8}, the average car density was set at 45 000 per day and the average car velocity 40 km.h^{-1}. The movement of cars causes the swirling of particles and exhaust gases. This phenomenon has great influence on the pollutants spread. Therefore the additional kinetic turbulent energy of value 9,3 $m^2.s^{-2}$ and dissipation rate of value 4,7 $m^2.s^{-3}$ were added in places around the volumes representing the exhaust [5].

Value of nitrogen dioxide concentration in case with additional kinetic turbulent energy can be seen in **Fig. 8**.

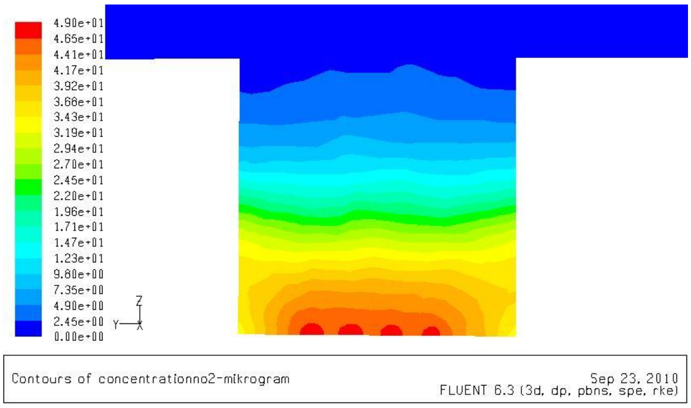

Fig. 8 Values of nitrogen dioxide concentration

Influence of the car body as resistance force [5] should also be included in the same area. The value of this force was computed, see equation (8) and set to the value 0,0004 $\mathrm{N \cdot m^{-3}}$ defined in Fluent.

$$\vec{F} = \frac{1}{2} \cdot \rho_{\infty} \cdot C_D \cdot A_p \cdot \left[\vec{U}_{\infty} - \vec{U}_{car}\right] \cdot \left(\vec{U}_{\infty} - \vec{U}_{car}\right) \tag{8}$$

where:

ρ_{∞} –air density $[\mathrm{kg \cdot m^{-3}}]$,

C_D –shape coefficient $[-]$,

A_p –projection of the surface in the direction of fluid accrued $[\mathrm{m^2}]$,

$\vec{U}_{\infty}$ –vector of air velocity $[\mathrm{m \cdot s^{-1}}]$,

$\vec{U}_{car}$ –vector of cars velocity $[\mathrm{m \cdot s^{-1}}]$.

The resulting concentrations of nitrogen dioxide can be seen in **Fig. 9**.

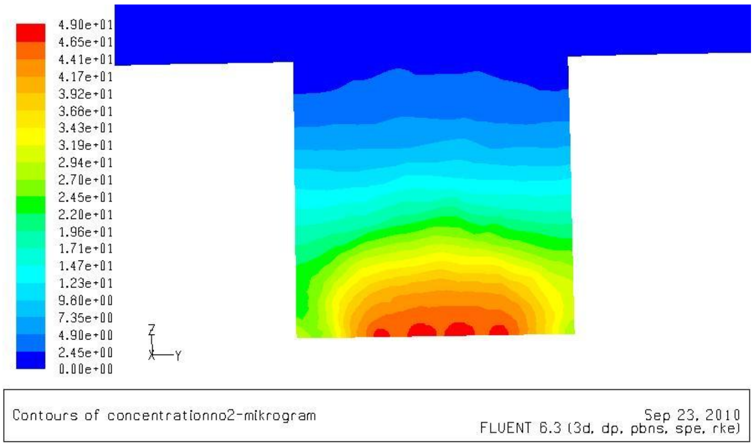

Fig. 9 Values of nitrogen dioxide concentration - additional force

CONCLUSION

The approach used in tested procedure of simplified street canyon will also be applied in the simulation of pollutant concentration in Leger street and compared with experimental measurements.

The results show that the resistance forces and additional turbulent kinetic energy caused by moving car body must be included in mathematical model to obtain high-guality nitrogen dioxide concentration.

The intensity of solar radiation was not included in these simulations. In autumn and winter solar radiation intensity is not so important, therefore, the resulting values can be regarded as identical. Another situation comes up in the summer months especially. In those cases it would be necessary to keep in mind that solar radiation strongly affects the chemistry of the atmosphere.

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