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VERIFICATION OF OPEN SOURCE CFD SOFTWARE PACKAGE OPENFOAM AGAINST THE MUST WIND TUNNEL EXPERIMENT ON ATMOSPHERIC DISPERSION

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Introduction. Modeling of air pollution in urban areas is one of important and actual problems of modern ecology. In close proximity to buildings the application of Gaussian models is not justified. There is a need for use of the models allowing solving the full system of the hydrodynamic equations. This allows receiving the correct values of pollution at close distances to the buildings. Such calculations require significant computational resources and this imposes additional requirements to the used model:

- ability to modify the program code; it allows to simplify system of the equations and to consider characteristic features of the solved task;
- the ability to use unstructured mesh; it allows to refine a mesh in the necessary places instead of use of the refined mesh in all the computational domain;
- the possibility of parallel computing; it allows to use possibilities of multicore architecture of modern clusters.

The software package OpenFoam [1] meets all these requirements. The OpenFOAM [1] (Open Field Operation and Manipulation) CFD Toolbox is a free, open source CFD software package which is extensively used across most areas of engineering and science. OpenFoam is a C++ toolbox for the development of customized numerical solvers, and different utilities for the solution of continuum mechanics problems, including computational fluid dynamics (CFD). The purpose of this work is verification of the OpenFoam CFD code against the data of the MUST wind tunnel experiment on distribution of pollution in urban areas.

Description of the MUST experiment. The Mock Urban Setting Test (MUST) was a large international field experiment, which was carried out on a test site of the US Army in the Great Basin Desert in 2001 [2]. The wind tunnel experiment [3] carried out at the Environmental Wind Tunnel Laboratory at Hamburg University has been scaled for the conditions of the field MUST experiment with the scale factor 1:75. Verification of the OpenFOAM in this work was carried out for the wind tunnel experiment which is hereafter also refereed as ‘MUST experiment’.

In the MUST experiment total of 120 standard size shipping containers were set up in a nearly regular array of 10 by 12 obstacles. The containers were nearly identical and were on average 12.2 m long, 2.54 m high and 2.42 m wide with the only exception from the standard size container is a so-called VIP car (container code H5) near the center of the array. The contaminant’s concentration has been measured by an array consisting of 256 detectors. Height of measurements for all concentration detectors was 1.28 m. A point source is located at the ground level with volume flow rate of gas: $\approx 3.3 \times 10^{-6}$ m^3/s. Meteorological sensors located at different levels cover that part of the computational domain were arrows are shown in Fig. 1 (hereafter refereed as ‘coarse sensors grid’). The aerial density of meteorological sensors is much higher in part of the domain shown by the blue square (hereafter refereed as ‘fine sensors grid’)

This study is limited to a single meteorological event: neutral stratification, wind speed 8 m/s at the roof level 7.29 m, the wind direction -45 degrees. Measured wind profile was close to the logarithmic profile with a roughness length equal to 0.0165 m.

The model equations and numerical schemes. Calculation of a wind speed distribution around buildings was performed by a solution of the stationary Reynolds-averaged equations of hydrodynamics of incompressible liquid, without taking into account heat exchange processes. In simulations the standard k-ε model was used. To solve these equations we used the standard steady-state solver simpleFoam, for incompressible, turbulent flow, from the software package OpenFOAM [1].

Pollution transport is calculated separately from the hydrodynamic equations using the already obtained wind speed distribution and turbulent diffusion coefficients. The stationary equation of scalar transport was solved. In more detail the used equations and their implementation in Openfoamis described in [4].

In the created model of MUST experiment there are three different physical types of bounding surfaces:

- the two opened vertical boundaries through which the wind blows in computational domain and the top side – are described by means of a Dirichlet boundary condition; the standard logarithmic profile of a wind was used;
- the two opened vertical boundaries through which the wind blows from the computational domain – are described by means of a Neumann boundary condition (gradient is equal to zero);
- the walls of the containers and bottom surface were considered as aerodynamically smooth surfaces.

Approximation of the convective term in meteorological calculations was executed by means of the well-known first-order upwind scheme. For the solution of the transport equation the second order of accuracy schemes were used.

In the calculations we used three different meshes: coarse, middle and fine. All calculations were executed on the coarse mesh at the beginning. The received results were interpolated to the middle mesh and thereafter from middle to the fine mesh. For interpolation volume fields from one mesh to another mesh the standard OpenFOAM utility mapFields [1] was used. Calculations with different grid resolution allows significant acceleration of computations for a fine grid and it allowed to execute Richardson extrapolation [5], for calculation the grid-convergent results.

Verification results. Statistical indicators of errors of wind speed and wind direction are given in Table 1. Errors are given for two sets of sensors (coarse and fine sensors grid) and all heights where measurements were taken.

Table 1 Errors of wind speed and wind direction for a coarse sensor grid at the different levels ME=<Fo-Fp> – mean error, MAE=<|Fo-Fp|> – mean absolute error, RMSE=$<(Fo-Fp)^2>^{0.5}$ – root mean square error. Indices 'o' and 'p' stay for observation and prediction

Height, m	WS/ Uref			WD		
	ME	MAE	MSE	ME	MAE	MSE
1.275	0.14	0.16	0.19	10.03	12.43	17.86
2.55	0.16	0.16	0.19	3.31	5.88	8.46

Figure 1 shows the measured and calculated fields of wind at two height levels for the coarse sensors grid. For the more exact representation of local processes in close proximity to buildings, in Figure 2 the field of the measured and calculated winds for a fine grid of meteorological sensors is presented.

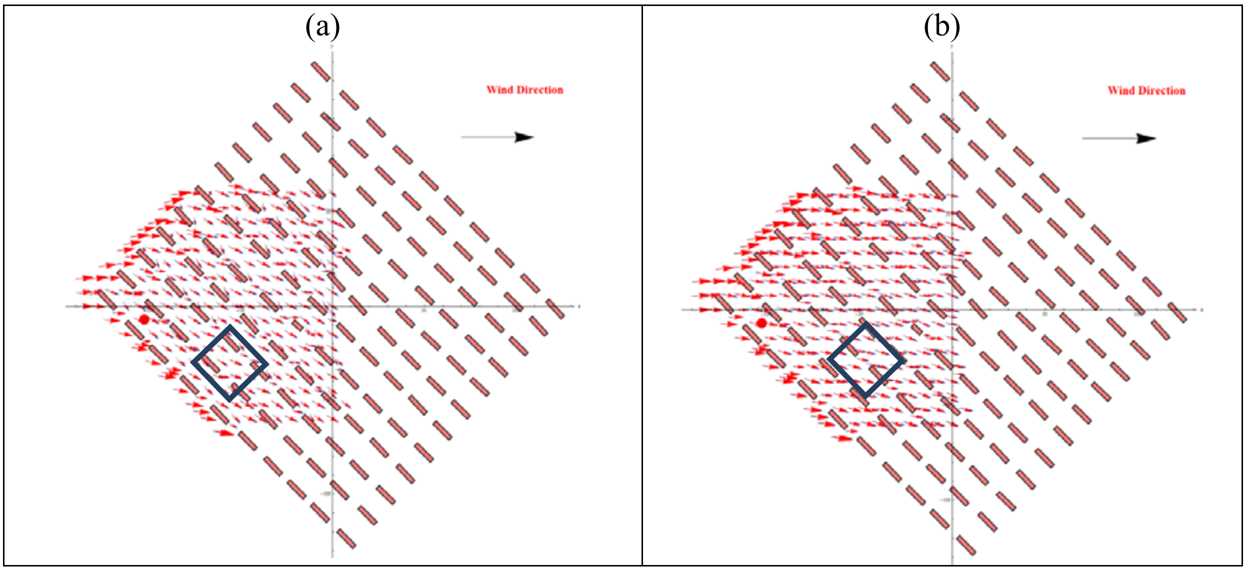

Figure 1. The measured (blue arrows) and calculated (red arrows) wind fields on a coarse sensor grid at two levels. Left picture corresponds to level 1.275 m, right – level 2.55 m. The blue line limits a fine grid of sensors

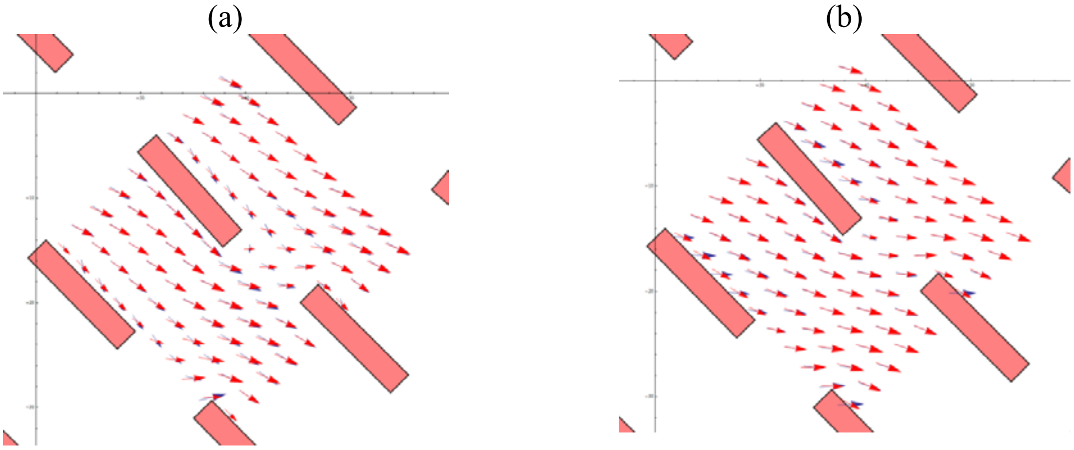

Figure 2. The measured (blue arrows) and calculated (red arrows) wind fields on a fine sensor grid at two levels. (a) –1.275m, (b) –5.75 m

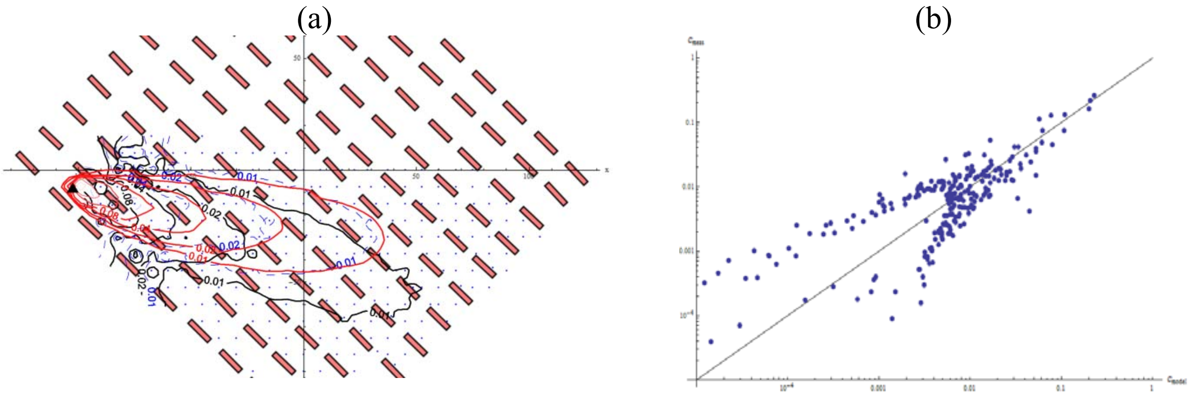

Figure 3. (a) Isolines of the calculated and measured fields of concentration. (b) Scatter plot of the calculated vs measured concentrations

The field of concentration at the height of 1.28 m and comparison of the calculated concentration with the measured is presented in Figure 3. From the above illustrations it is seen that the calculated and measured fields are characterized by the comparable values. However the calculated concentration distribution to less extend deviates from the reference wind direction as compared to measured distribution.

Summary of the statistical results of of the calculated concentrations for three runs with various spatial resolution are given in Table 2. As it could be expected, mesh refinement improves the simulation result. Richardson's extrapolation allowed to find grid-convergent value and to estimate the smallest possible error which could be obtained with this model.

Table 2 Errors of concentration for the three different spatial resolutions and the result of Richardson extrapolation

Number of cells		
N1	10259775	
N2	1249305	
N3	145185	
Refinement ratios		
r21	2.000	
r32	2.048	
	Normalized mean square error $NMSE = \frac{\overline{(C_0 - C_p)^2}}{\overline{C_0} \times \overline{C_p}}$	**Fractional bias** $FB = 2 \times \frac{\overline{C_0 - C_p}}{\overline{C_0} + \overline{C_p}}$
ϕ_1	0.577	-0.011
ϕ_2	0.751	−0.075
ϕ_3	1.329	−0.085
ϕ_{ext}^{21} (Richardson-extrapolated)	0.495	0.0006

Conclusions. Verification showed that the CFD code OpenFoam is the convenient and flexible tool for modeling of atmospheric dispersion and transfer of pollution in a neighborhood urban buildings. The given approach, allows to reproduce with satisfactory accuracy the meteorological fields and to simulate atmospheric transport of the pollutants with the acceptable accuracy. The obtained statistical characteristics of errors are in admissible range and are comparable with the results of other widely known models [6]. Perhaps the choice of optimum model of turbulence and use of numerical schemes of a high order will improve the results. It is material for future researches.

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