ROUZ CODE: CFD APPROACH FOR ASSESSMENT OF RADIATION SITUATION DURING ATMOSPHERE RADIOACTIVITY RELEASES WITHIN AN INDUSTRIAL SITE

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Abstract. According to the state-of-the-art trends in applied computational meteorology a robust CFD model has been developed in the IBRAE RAN. The V&V matrix of the ROUZ code contains various data obtained from real emergency cases as well as gathered from experiments conducted in urban conditions and at industrial sites, for example, experiment in Oklahoma City. It is demonstrated that ROUZ code satisfies the quality acceptance criteria defined by the expert community for models of the same class.

Key Words: Microscale meteorological models, passive tracer transport, dose calculation.

A distinguishing feature of the modern approach to modelling of contamination transport for industrial and urban areas is that it takes into account 3D flows around buildings. As a result, an opportunity appeared to account for aerodynamic effects and obtain more realistic pollutant concentration distributions than within traditional gaussian approaches.

Microscale meteorological models which calculate meteorological parameters within industrial and urban areas have been actively developed in the last few years [1]. Models based on LES and DNS approaches are used in theoretical studies. Practical applications are, as a rule, restricted to RANS models.

These models in turn, divided into special-purpose (MISKAM [2], FE3MP [3]) and general purpose codes. The former are characterized by the implementation of closure functions in the atmospheric surface layer (Monin-Obukhov theory). As opposed to general purposes code they do not require mesh refinement in the vicinity of underlying surface and buildings since the value of turbulent viscosity is calculated using the aforementioned closure model.

A robust CFD-RANS model called ROUZ has been developed in Nuclear Safety Institute (NSI) that allows to obtaining airborne and surface contamination fields as a result of gas and aerosol releases taking into account real geometry of buildings, atmosphere stability and inhomogeneous turbulence in the atmospheric boundary layer.

The model is based on the incompressible Navier-Stokes equations. Instead of using a wall-function approach the parametrisations of impulse and heat fluxes are utilized as described in the article [4].

In order to determine the friction velocity u^* on the surface the following relationship is used [4]:

$$u\left(z\right)=\frac{u^{*}}{\kappa}\left[\ln\left(\frac{z}{r}\right)-\left\{\ln\left(\frac{1+\xi^{2}}{2}\right)+2\ln\left(\frac{1+\xi}{2}\right)-2arctg\left(\xi\right)+\frac{\pi}{2}\right\}\right] \qquad (1)$$

where $\xi=\left(1-\frac{\gamma z}{L}\right)^{0.25}$;

z – the distance from the first computational mesh layer to the ground;

$\kappa = 0{,}41$ – Karman’s constant;

$\gamma = 15$;

r – the surface roughness;

L – the Obukhov length that depends only on the stability class of the atmosphere and is determined as follows:

$$L=\frac{r^{-\alpha}}{a} \qquad (2)$$

where the empirical coefficients depending on stratification are given in the work [4].

In order to determine turbulent heat fluxes $\overline{w'\theta'}$ parametrization (3,4) are used [5]. the following parametrizations are used in case of neutral and unstable stratification :

$$\overline{w'\theta'}=-u^{*}\frac{\theta^{BO3}-\theta^{3EM}}{\frac{R}{\kappa}\left(\ln\left(\frac{z}{r}\right)-2\ln\left(\frac{1+\eta^{2}}{2}\right)\right)} \qquad (3)$$

and for stable stratification:

$$\overline{w'\theta'}=-u^{*}\frac{\theta^{AIR}-\theta^{GROUND}}{\frac{R}{\kappa}\left(\ln\left(\frac{z}{r}\right)+\frac{\beta z}{RL}\right)} \qquad (4)$$

where $\eta=\left(1-\frac{\lambda z}{L}\right)^{0.25}$;

$R = 0{,}74$,$\lambda = 9$;

θ^{AIR} – the potential temperature of the air at the first computational layer

θ^{GROUND} – the temperature of the ground which is kept constant during the run of the code;

z – the distance from the first computational mesh layer to the ground;

w' – the fluctuating component of the vertical velocity;

θ' – the fluctuating component of the potential temperature.

The usage of such parametrizations limits the set of computational meshes that can be employed. The cell size of a mesh should not be less than 20-30 times the Obukhov length.

In all boundary cells the kinetic energy and the dissipation rate are given by the following expressions:

$$k = \frac{u_*^2}{C_\mu^{1/2}} \tag{4}$$

$$\varepsilon = \frac{u_*^3}{\kappa z} \tag{5}$$

Some results of verification and examples of ROUZ code application are given as follows.

As is shown by previous studies data sets obtained in experiments are not always valid for verification of models in use. This inspired the international scientific community to initiate creating data bases valid for verification of such models [6].

One can discern two approaches to a solution of this problem.

The first approach consists in creating verification data bases by assembling information from wind tunnel experiments. The second approach gives priority to verification against experiments conducted under natural atmospheric conditions [7].

Both approaches have their own pros and cons. In wind tunnel experiments it is very difficult to model some phenomena, such as: stratification, thermal effects as a result of heating or cooling building surfaces, chemical reactions and aerosol depositions.

A coarse measurement grid being characteristic of field experiments does not allow to accurately estimating the parameters of an inhomogeneous and unsteady flow in order to be used for comparison with the results of calculations.

At the present time there exist quantitative criteria of the quality of the results obtained by microscale meteorological models. In the literature the results of modelling are mainly represented via usage of two quantitative criteria.

In order to verify ROUZ code we estimated the quality of modelling employing the following criteria [1]:

- FA2 (factor of 2 of observation), counts the fraction of data points for which the following relationship holds true

$$FA2 = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i \text{ where } N_i = \begin{cases} 1 \quad when \quad \frac{1}{2} \le \frac{C_{calc}}{C_{obs}} \le 2 \\ 1 \quad when \quad C_{obs} \le W \quad u \quad C_{calc} \le W \\ 0 \end{cases} \tag{6}$$

- Hit Rate is defined as

$$q = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i \quad \text{where } N_i = \begin{cases} 1 \quad when \quad \left|\frac{C_{calc} - C_{obs}}{C_{obs}}\right| \le D \\ 1 \quad when \quad \left|C_{calc} - C_{obs}\right| \le W \\ 0 \end{cases} \tag{7}$$

where C is a variable (either a component of velocity or concentration);

n is a total number data points;

N is the fraction of computational nodes where values of the variable are regarded as close to measured values.

Parameter D accounts for the relative uncertainty of comparison data while W reflects the degree of experimental uncertainty. The magnitude of D is equal to 25% for all runs, according to [8,9]. The magnitude of W is determined via statistical analysis of the scatter of measured variables obtained in a series of experiments conducted under the same conditions.

Within the framework of the project COST732 was created a data base called CEDVAL [1] (Compilation of Experimental Data for Validation of Microscale Dispersion Models) consisting of a set of wind tunnel experiments. The geometry of obstacles varied from a single rectangular obstacle to buildings with a slanted roof and an arranged array comprising 21 buildings.

The results of verification against the CEDVAL experiments data including about 9000 data points is given in table 1 in the form of the aforementioned metrics.

A result of comparison for each component of velocity is a sum of the metrics in all experiments. Each metrics is introduced into the sum with a relative weight equal to the relation of the number of data points in the experiment to the number of measurement points in all experiments.

TABLE I: SUMMARY OF RESULTS FOR ALL COMPONENTS OF VELOCITY IN ALL EXPERIMENTS.

Criterion	**Result**
FA2 (U)	87%
FA2 (V)	96%
FA2 (W)	93%
Hit rate (U)	76%
Hit rate (V)	82%
Hit rate (W)	75%

The values of quality acceptance limits for Hit Rate and FA2 metrics are equal to 66% and 55% accordingly. These values are applied for quantitative analysis of microscale meteorological models in accordance with COST732 documentation.

In addition to laboratory experiments a comparison between modeled and measured values of concentration was made using the data of Joint URBAN 2003 field experiment (the center of Oklahoma-city).

The locations of the source of passive tracer and of measurement points are shown in *FIG. 1.*

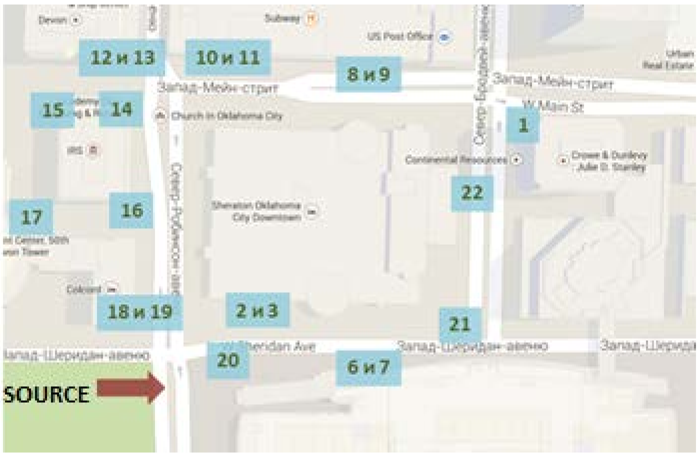

FIG. 1. Release point and measurement stations.

FIG. 2. compares ROUZ model concentration field with experimental values obtained at the measurement stations. Green squares denote ROUZ model results, blue triangles stand for values measured at stationary measurement grid.

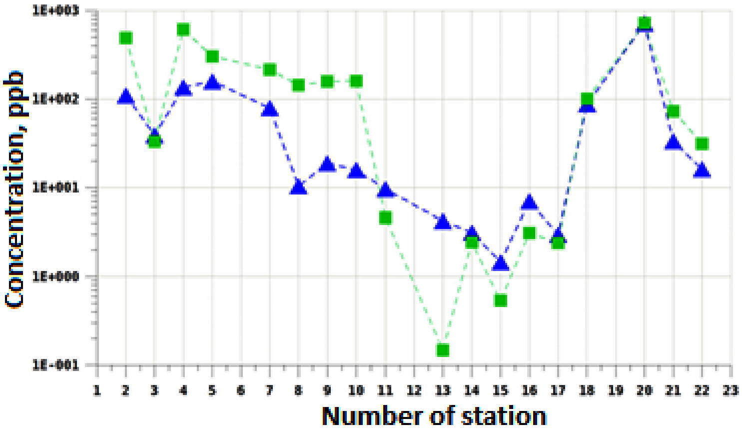

FIG. 2. ROUZ model results against experimental values.

Contamination fields in the streets of a real city are very complex. The increase in concentration in near points can be of three orders of magnitude. A significant discrepancy is indicated by station 13, where model results are undervalued in comparison with that of measured. Nonetheless, the absolute maximum of concentration (measurement station 20) matches model results with a relative accuracy of 5%.

Let us gain insight into a situation related with measurement station 13 where the largest discrepancy was observed. In *FIG. 3.* the location of that station (and station 14) is shown, as well as isolines of model concentration of tracer in that area. One can observe that contamination field in that area is strongly inhomogeneous and horizontal gradient is high. Hence, the value of concentration of contamination in the vicinity of point 13 is significantly larger than in the point itself.

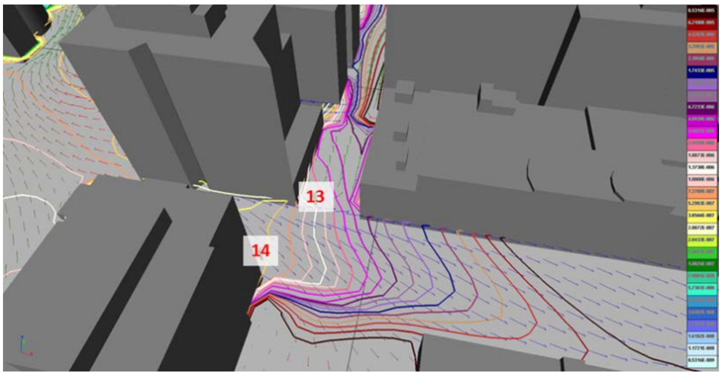

FIG. 3. Isolines of surface concentration in the vicinity of station 13 and 14.

Apart from calculations of fields of contamination code ROUZ performs shielding calculations of doses received from a plume of arbitrary shape based on the assumption that large buildings incorporated into a model an industrial facility completely absorb considered radiation.

An example of usage of code ROUZ for contamination filed modelling for the area near Beloyarskya NPP under an accident scenario is shown in *FIG.4.*

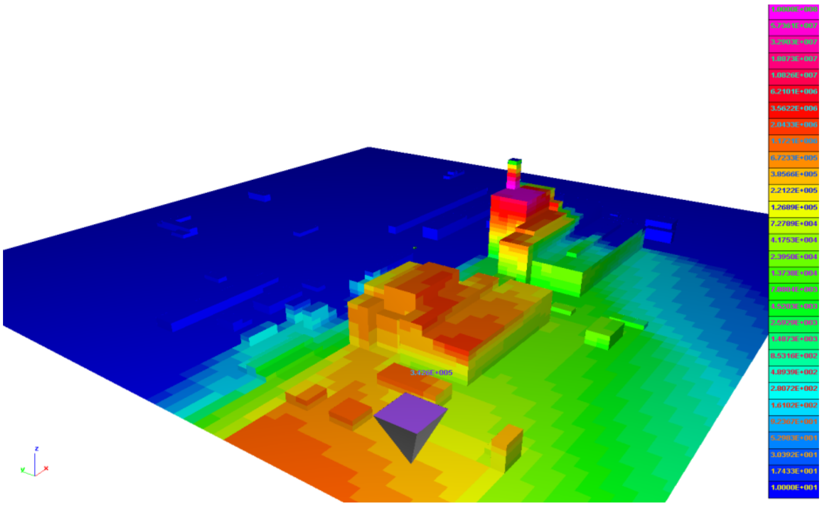

FIG. 4. Visualization of a concentration deposition field in the area of Beloyarskaya NPP.

Therefore, verification of ROUZ code against international bases data demonstrated that code ROUZ meets the quality criteria the specified by the international science community [7].

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