# Atmospheric dispersion modelling over coal mine excavation – on LES validation by wind-tunnel experiment

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ABSTRACT

Results from validation of large eddy scale simulation model (LES) by wind-tunnel experiment are presented. The neutrally stratified atmospheric dispersion over real complex terrain – open-cut coal mine with necessary surroundings – was simulated in order to predict the air quality in populated areas situated close to the coal mine with respect to prevailing wind direction. As a computational model the LES numerical model Charles University Large-eddy Microscale Model (CLMM) was used. For wind-tunnel experiment the simultaneous point measurement of two velocity components and concentrations by Laser Doppler Anemometry (LDA) and Fast Flame Ionization Detector (FFID), respectively, was performed. The mean velocity and concentration field obtained from wind-tunnel measurements are compared qualitatively with those from LES by means of Hit Rate and FAC2 (Factor of two observations) metric, respectively. According to metrics thresholds (both Hit Rate and FAC2 must be higher than 60%) and recommended metric parameters (allowed absolute and fractional deviation is $W \leq 0.05$ and $D \leq 0.25$, respectively) the LES model was successfully validated with respect to dimensionless longitudinal velocity component and concentration. For all 6 investigated vertical planes the Hit Rate and FAC2 mean was 93% and 76 %, respectively, for mentioned quantities. In case of dimensionless vertical component the low Hit Rate mean of 19% providing allowed absolute deviation $W = 0.002$ is discussed. Considered the most important result both LES and experiment confirm the highest concentration values capture at the coal mine excavation.

## 1 INTRODUCTION

The open-cut coal mine situated in the north-west of Czech Republic represents a pit of huge dimensions (approx. 5km long, 4km wide and 115m deep). If we want to observe the pollutant dispersion processes in classical wind-tunnel utilized for atmospheric dispersion modelling the model results in very small scale (> 1:5000). The problems with two-phase flow modelling arise because many similarity criteria for dust emission modelling can't be met (e.g. threshold and terminal velocity ratio). Thus, the computational modelling could be very helpful for solving this kind of tasks, especially in case of hybrid approach (combining experimental with computational modelling).

Up to date the LES models were not applied for prediction of pollutant dispersion from open-cut coal mines. The last computational study concerning particulate emission from open pit quarry under neutral atmospheric conditions was presented by Silvester et al. (2009) where the commercial CFD software ANSYS FLUENT solving Reynolds-Averaged Navier–Stokes equations (RANS) by standard $k$-$\varepsilon$ model was used to simulate the airflow in and around the quarry. The transport of particulates from quarry was modelled using a Lagrangian particle tracking model, called the Discrete Phase Model (DPM). However, the comparison with experimental results was not presented.

For validation of LES model by means of quantitative metrics *Hit Rate* and *FAC2* (see more in Schatzmann (2010)) we used wind-tunnel experiment approach used only by Meroney and Grainger (1992) where the atmospheric dispersion of gaseous pollutant above the open-cut mine was simulated by helium/air tracer gas mixtures in the stratified flow. We decided to model neutrally stratified flow instead and simulate the point source representing the mining machine at the bottom of the mine (the most frequently used position) for which we used ethane as a tracer gas. Because of better diffusivity and lower density of ethane contrary to coal dust, we assume that we also modelled the highest atmospheric dispersion of possible pollutants from coal mine to its surroundings.

# 2 METHODS

## *2.1 Wind-tunnel experiment*

### *2.1.1 MODEL*

The picture of the model taken from wind-tunnel test section is presented in figure 1 (left). The model was designed according to necessary part of the coal mine topography (situated at the north-west of the Czech Republic) with respect to future coal mine expansion and surrounding populated areas (south part of town Chomutov, Droužkovice village). This resulted in total squared area of 1.5 x 1.5m (5 x 5 km at full scale) and scale ratio 1:3300.

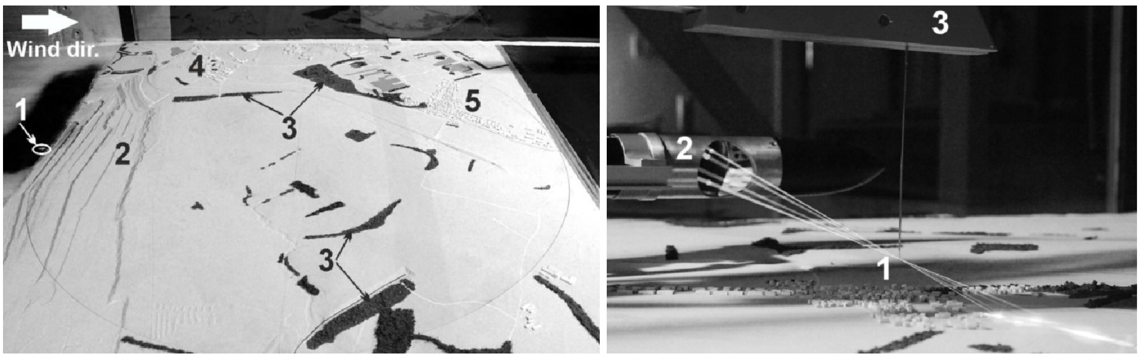


*Figure 1: Left: Model of scale ratio 1:3300 positioned at wind-tunnel including point source of pollutant (1) integrated at the bottom of special inclination smoothly connected to east end of coal mine (2), necessary vegetation (3), south part of town Chomutov (4) and village Droužkovice (5). Right: simultaneous point (1) measurements of two velocity components and concentrations by LDA (2) and FFID (3), respectively, above the model during measurements*

The model was made of extruded polyurethane and manufactured by computer numerically controlled (CNC) machine with precision of 0.5 mm. The special roughness of 0.5 mm was applied by CNC machine for model surface as well as all necessary vegetation and urban areas were made manually for completeness in order to fulfil the aerodynamic roughness of moderately rough terrain. As input data for CNC the geographic information system (GIS) was used.

### *2.1.2 MEASUREMENT TECHNIQUES*

The experiment was carried out at open Environmental wind-tunnel of Institute of Thermomechanics Academy of Sciences of the Czech Republic in Nový Knín. The tunnel is 1.5m wide and 1.5m high and consists of two main sections: 20m long section for development of appropriate boundary layer and following 2m long test section where the measurements above the model are performed. The wind-tunnel free stream speed can be maintained from 0.1 up to 13m/s. For our case of small scale ratio (1:3300) the development section was kept empty without any roughness elements and spires. Only 1.5m of special inclination smoothly connected to model relief was kept in development section. This special inclination reproduces topography of coal mine situated in front of the modelled area and was roughen by sand grains (size of the grains was smaller than 0.5mm) in order to achieve aerodynamically rough flow and appropriate characteristics of modelled atmospheric boundary layer.

In figure 1 (right) is presented the unique method used for simultaneous point measurements of two velocity components and concentrations by two-dimensional optical fibre Laser Doppler Anemometry (LDA) and Fast-response Flame Ionization Detector (FFID), respectively, developed by Kukačka et al. (2012). We used ethane as a tracer gas simulating passive pollutant releasing from point source positioned at the bottom of the coal mine. The wind-tunnel free stream velocity was measured by Prandtl tube at fixed position in the centre of wind-tunnel 3m in front of the model and 0.9m above the floor and was used as a reference velocity $u_{ref}$ for point measurements.

### *2.1.3 Boundary layer*

Two–dimensional LDA measurements for obtaining characteristic vertical profiles were performed above the centre of the special inclination (in front of the model entrance) using a reference wind speed $u_{ref}$ = 5.2 m/s. Measured vertical profile of dimensionless mean longitudinal velocity $u/u_{ref}$, turbulence profiles and turbulence spectra are compared with those from VDI guidelines in figure 2. Mean roughness length $z_0$ = 0.04 m (converted to full scale) and power exponent α = 0.13 was obtained from the log fitting and power fitting, respectively. According to VDI (2000) for moderately rough terrain the $z_0$ should be from $5.10^{-3}$ to $10^{-1}$m and $\alpha$ from 0.12 to 0.18.

The turbulence spectrum was evaluated at four heights of measured vertical velocity profile: 13.5, 57, 100 and 600m (full scale) above the inclination surface. The spectra for height 100m were compared with Kaimal, Karman and Simiu&Scanlan spectra in figure 2 (right). The best fit of measured spectra is with the Karman spectra for all four heights.

According to these comparisons we can conclude that boundary layer for moderately rough type of terrain was modelled appropriately. Furthermore, the Reynolds number, averaging time and source strength independence was fulfilled as well.

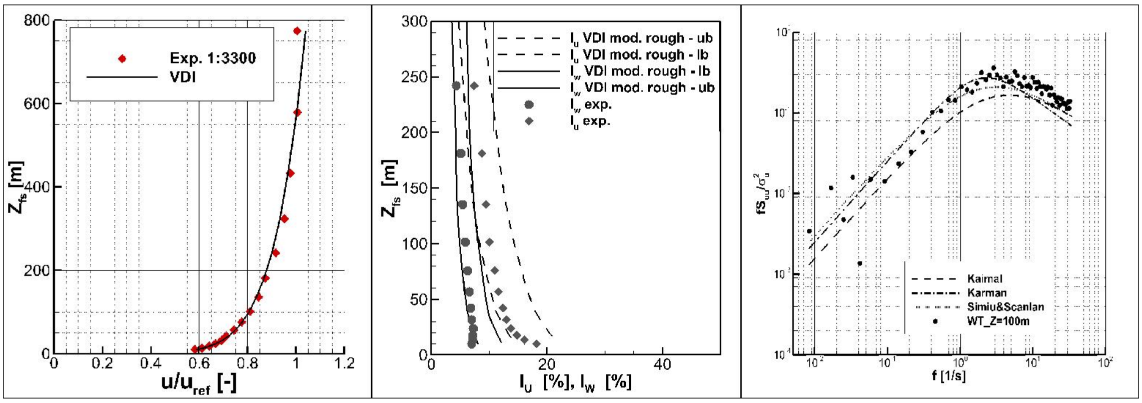


*Figure 2: The vertical profile of dimensionless longitudinal velocity $u/u_{ref}$ (left), vertical profiles of turbulence intensities $I_u$, $I_w$ (middle) and longitudinal velocity turbulence spectrum $S_{uu}$ of modelled boundary layer at full scale height 100m above the terrain (WT_Z=100) compared with Kaimal, Karman and Simiu&Scanlan spectra (right).*

## *2.2 Computational model*

The numerical model CLMM (Charles University Large-Eddy Microscale Model) solves the equation of fluid dynamics and scalar transport under the assumptions of the large-eddy simulations. Mathematical description of its dynamical core is available in Fuka and Brechler

(2011). In addition to this reference, the fourth order central method for momentum advection and a discrete filter to non-linear terms have been applied. The model uses the uniform Cartesian grid and the immersed boundary method to account for the complex terrain. The resolution of the computational grid was $\Delta x = \Delta y = 5.9$ mm and $\Delta z = 1.5$ mm (according to scale of wind-tunnel model).

For simplicity, the periodic boundary conditions were used at the domain boundaries in horizontal directions. The terrain was made periodic by solving the Laplace's equation with the periodic boundary conditions on domain boundaries and the Dirichlet boundary conditions at the real terrain boundaries. The whole computer model terrain elevation map including the periodicity buffer regions is in figure 3.

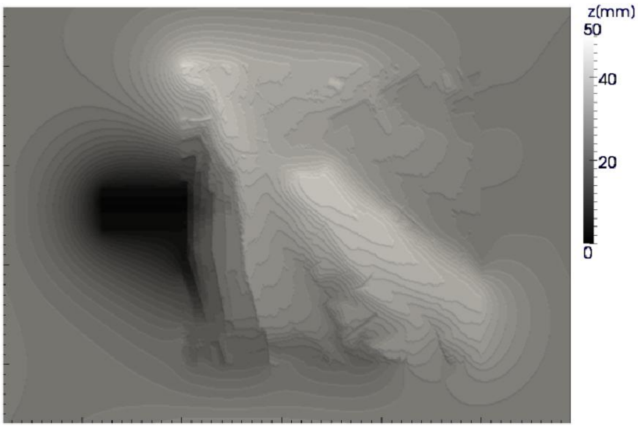


*Figure 3: The elevation map of the simulated domain. The steps both in vertical and horizontal directions correspond to the resolution of the computational grid.*

## 3 RESULTS

The LES validation was investigated at 6 vertical planes as depicted on model contour map in figure 4: five planes perpendicular (*yz*) and one plane parallel (*xz*) with approach wind direction. The measured planes are investigated at dimensionless coordinates *x/h, y/h* and *z/h* where *h* is a coal mine depth (*h* = 35 mm, corresponding to 115m at full scale).

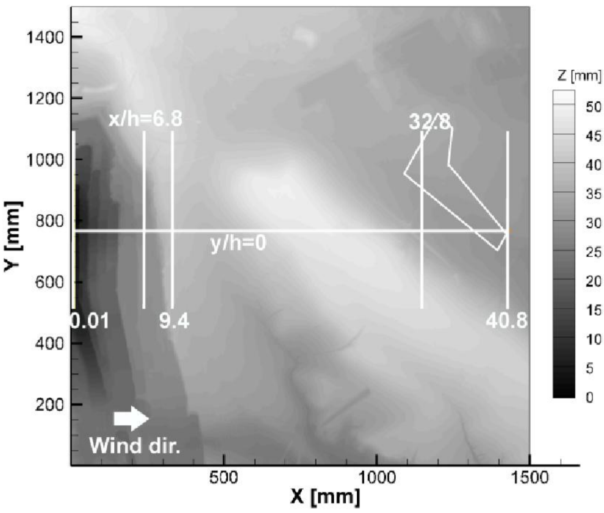


*Figure 4: Measured 5 vertical planes yz (vertical lines – x/h) and one vertical plane xz (horizontal line – y/h) displayed on model contour map. Approach wind direction is from left to right. Note the elongated hill in the middle of the model (white contours) and coal mine escarpments (the most left in the picture).*

### 3.1 Qualitative comparison

For the first examination of LES model validation the some qualitative comparison of velocity and concentration fields from LES and experiment are presented in figure 5 and 6, respectively.

#### 3.1.1 VELOCITY FIELD

In the upper part of the figure 5 are plotted the mean dimensionless longitudinal velocities $u/u_{ref}$ from LES (left) and experiment (right) at plane parallel with approach wind direction positioned at the point source origin ($y/h$ = 0). In the lower part the mean dimensionless vertical velocities $w/u_{ref}$ are compared. We can see very good "visual" agreement between LES and experiment in both longitudinal and vertical velocity field.

#### 3.1.2 CONCENTRATION FIELD

Dimensionless concentration field from both LES and wind-tunnel experiment at the same plane as in case of velocity fields (*xz*) is presented in figure 6. As in previous case the concentration fields are very similar (the highest concentration levels are kept within coal mine excavation). But, the exact values cannot be determined explicitly (from both velocity and concentration fields comparison), hence the qualitative comparison tells us only approximate results in case of velocity and concentration filed comparison.

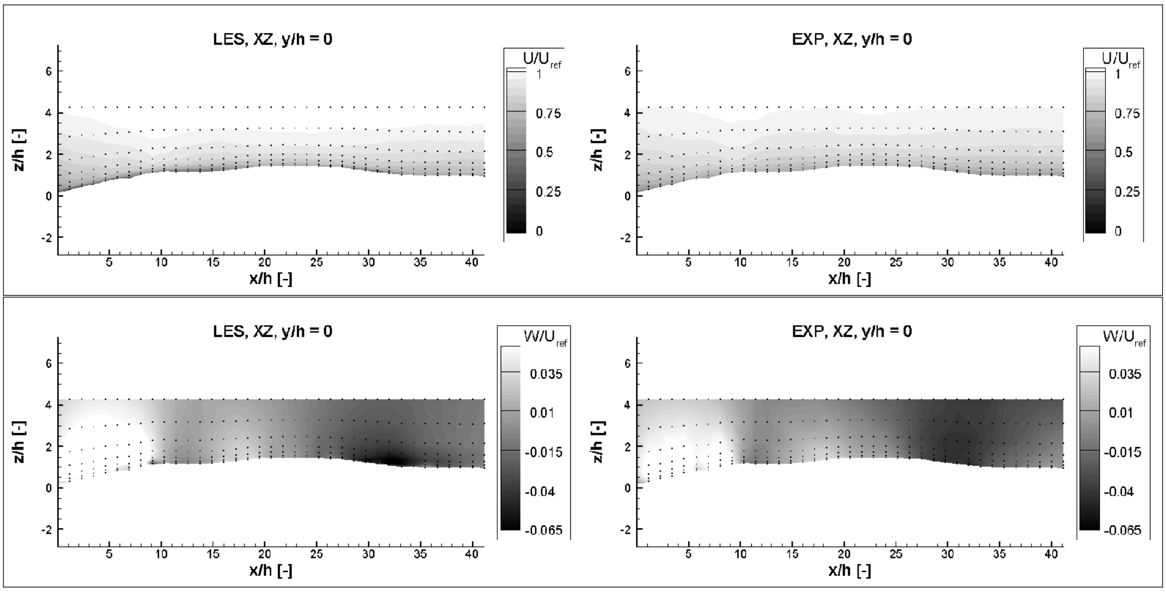


*Figure 5: Comparison of LES (left) and wind-tunnel (right) mean dimensionless longitudinal $u/u_{ref}$ (up) and vertical (down) velocities $w/u_{ref}$ at plane xz parallel with approach wind direction positioned at the point source origin (y/h = 0).*

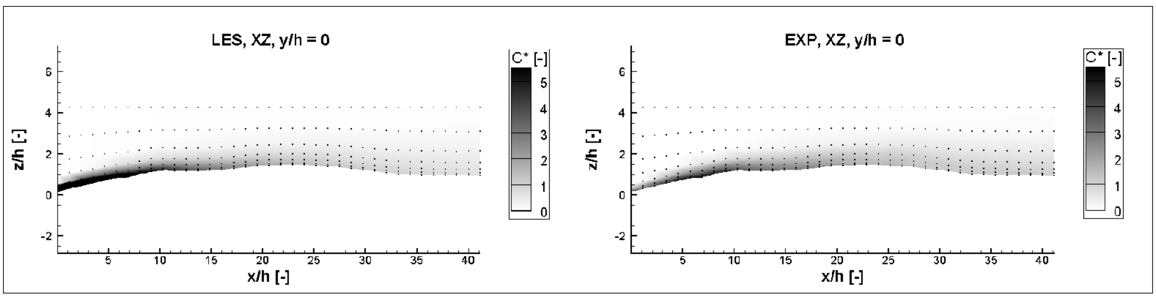


*Figure 6: Comparison of LES (left) and wind-tunnel (right) mean dimensionless concentrations C* at plane xz parallel with approach wind direction positioned at the point source origin (y/h = 0).*

### 3.2 *Quantitative comparison*

To have better insight into LES validation the quantitative comparison based on validation metrics (*Hit Rat*e and *FAC2*) is presented and discussed in this chapter. Generally speaking the validation metrics help to quantify the agreement between the numerical simulation and experimental data.

#### 3.2.1 *Hit Rate*

For velocity validation we used the *Hit Rate* (*q*) metric, applied in VDI (2005) on prognostic micro-scale wind field model, defined by following equation:

$$q = \frac{N}{n} = \frac{1}{n}\sum_{i=0}^{n} N_i \text{ with } \begin{cases} 1 \text{ for } \left|\frac{P_i - O_i}{O_i}\right| \le D \text{ or } |P_i - O_i| \le W \\ 0 \text{ else} \end{cases} \qquad (1)$$

$P_i$ (predicted) represents normalised model result and $O_i$ (observed) normalised result from experiment. The equation (1) specifies the fraction of the model results that differ within an allowed range of *D* or *W* from the comparison (here experimental) data. *D* accounts for relative uncertainty and *W* the repeatability of the experimental data. According to VDI (2005) *D* was always 25% ($D = 0.25$) but *W* should be different for each variable with respect to the experimental uncertainty (Schatzmann et. al (2010)). The threshold for successful validation is $q >$ 0.66 (i.e., $q >$ 66%). For an ideal model prediction $q = 1$.

In figure 7 are presented scatter plots and *Hit Rates* for $u/u_{ref}$ (left) and $w/u_{ref}$ (right) at plane *xz*. It's worth to remind that this plane goes through the whole model. The *Hit Rate* in case of $u/u_{ref}$ is 93% for $D = 0.25$ and $W = 0.002$ and 32% in case of $w/u_{ref}$ for $D = 0.25$ and $W = 0.005$ (*W* was obtained from statistical scatter of the experimental values). Whilst *Hit Rate* for $u/u_{ref}$ is in very good agreement with qualitative comparison we cannot say the same for $w/u_{ref}$ because only third of total hits were achieved. From distribution of the points (red dots) is clearly seen that LES model slightly underestimates the lower values of $u/u_{ref}$. However, the scatter plot for $w/u_{ref}$ is even along the ideal hit (solid line splitting the quadrants on even parts). This also helps to explain why the qualitative comparison represents nice results for the first glance.

In figure 8 (left) is presented the scatter plot of relative turbulence kinetic energy $TKE/(u_{ref})^2$. Even though the $W = 0.001$ the *Hit Rate* is 81%. From points distribution we can see that LES slightly overestimates the *TKE*.

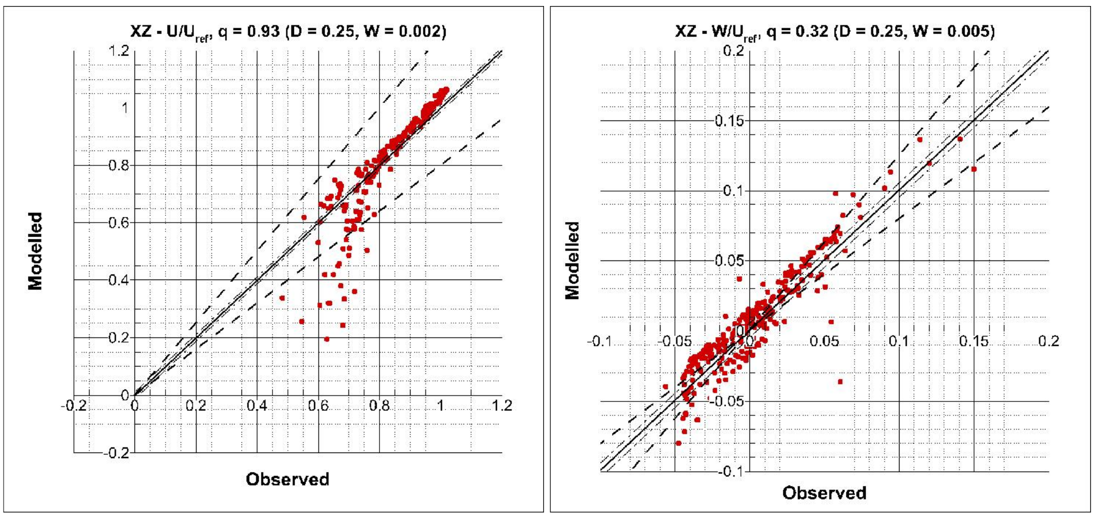


*Figure 7: Scatter plots and Hit Rates for $u/u_{ref}$ (left) and $w/u_{ref}$ (right) at plane xz. Dashed lines represent D and dash-and-dot W. Red points that are within these lines are counted as hits ($N_i = 1$).*

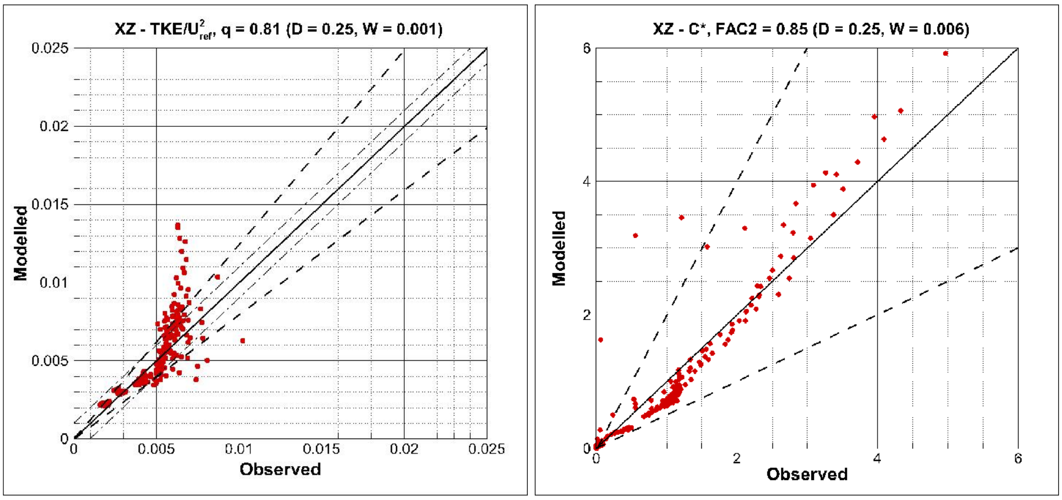


*Figure 8: Scatter plots of TKE/$u_{ref}$ (left) and C*(right) at plane xz. Dashed lines represent fractional deviation D and dash-and-dot absolute deviation W. Red points that are within these lines are counted as hits ($N_i$ = 1). For C* the FAC2 metric was used.*

For 5 investigated *yz* planes perpendicular to approach wind direction the following statistics of *Hit Rate* metric were observed (scatter plots are not presented): the lowest *Hit Rate* values 88%, 3 % and 75% for planes at the vicinity of last coal mine escarpment (*x/h* = 6.8 and *x/h* = 9,4, respectively) and the *Hit Rate* means 93%, 19% and 76% of all investigated planes for $u/u_{ref}$, $w/u_{re}$ and $TKE/(u_{ref})^2$respectively. The parameters *D* and *W* for the investigated variables were kept same as for plane *xz*.

### 3.2.2 FACTOR OF TWO OBSERVATIONS (FAC2)

For concentration validation the metric *FAC2* defined by Schatzmann et. al (2010) was used:

$$FAC2 = \frac{N}{n} = \frac{1}{n}\sum_{i=0}^{n} N_i \text{ with } \begin{cases} 1 \text{ for } 0.5 \le \frac{P_i}{O_i} \le 2.0 \\ 1 \text{ for } O_i \le W \text{ and } P_i \le W \\ 0 \text{ else} \end{cases} \qquad (1)$$

*FAC2* is similar to the *Hit Rate* as it counts the fraction of data points, where the predictions are within a factor of two of the observations, based on the ratio of the predicted and observed value. It is the most robust measure concerning the influence of infrequently occurring high or low observations and predictions for the concentrations. The *FAC2* threshold is same as for *Hit Rate*.

The scatter plot of dimensionless concentrations *C** and *FAC2* metric for plane *xz* are presented in figure 8 (right). We can see that 85% of the points are within the lines defining parameter *D* = 0.25 and *W* = 0.002. Distribution of the points is even along the ideal *FAC2* (solid line).

Decreasing tendency of *FAC2* with increasing distance from the point source was observed from 5 investigated *yz* planes as well as following statistics: the lowest *FAC2* value 50% at the last plane (downstream from the point source) and the *FAC2* mean 87% of all investigated planes providing the same parameters (*D* and *W*) as for plane *xz*.

## 4 CONCLUSIONS

The successful validation of LES model by means of quantitative comparison where for mean velocity and concentration field the *Hit Rate* and *FAC2* metric was used, respectively, was presented with following remarks.

Quantitative comparison demonstrates the misleading interpretation of results from qualitative comparisons, especially in case of vertical velocity field. For 5 investigated vertical planes perpendicular to approach wind direction the *Hit Rate* and *FAC2* mean was 93% and 87 % in case of mean dimensionless longitudinal velocity and concentration, respectively, confirming well appeared qualitative comparison. However, in case of vertical velocity field the highest *Hit Rate* 41% and *Hit Rate* mean 19% for all investigated planes was obtained contrary to well appeared qualitative comparison.

The lowest *Hit Rate* values in case of all variables were obtained for planes situated at the vicinity of last coal mine escarpment, pointing to problems with computational flow modelling around sharp edges. From observed decreasing tendency of *FAC2* with increasing the distance from point source the LES slight underestimation of concentrations at remote area can be stated.

Nevertheless, both LES and experiment revealed the same important effect of complex terrain topography and surface roughness on pollutant dispersion – the highest concentration values are kept within the coal mine excavation.

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