# Modelling of concentration fluctuations

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Keywords: concentration, fluctuations, modelling, wind tunnel, street canyon.

## 1 Introduction

The dispersion of a gaseous pollutant released in the atmospheric boundary layer has a strong random component due to the stochastic nature of turbulence. The fluctuations exhibited in the time series of measured concentrations are often of the same order of magnitude as the mean concentration.

The mean concentration field, defined either as time or ensemble average, is not adequate for estimating the potential hazards from releases of pollutants into the atmosphere. Toxicity and/or flammability of many gases depend on short-term concentration levels. Furthermore the evaluation of an atmospheric dispersion model, by comparison of the predictions with observations, requires the estimation of the model's uncertainty. The above can be achieved by calculating the magnitude of turbulent fluctuations of concentration.

Along these lines a computational model for concentration fluctuations has been formulated. In this article, computational simulation of a wind tunnel experiment of passive gas dispersion in a complex street canyon configuration provides a first step evaluation of this model.

## 2 Modelling approach

A transport equation for the concentration fluctuations has been formulated and introduced in the code ADREA-HF which is developed by the Environmental Research Laboratory. The purpose of ADREA-HF is to simulate the dispersion of buoyant or passive pollutants over complex geometries. The abovementioned transport equation adopts a gradient transport hypothesis with an eddy diffusion coefficient for closing the turbulent terms of production and diffusion. The eddy diffusivity is assumed equal to the eddy diffusivity for concentration and is calculated by a 1-equation  $k-l$  model for the turbulent kinetic energy. The eddy dissipation term is calculated using the turbulent kinetic energy and a length scale, equal to some characteristic cloud height or the turbulent length scale. Detailed description of the model can be found in Andronopoulos et al. (1993).

## 3 Wind tunnel experiments

The Environmental Flow Research Centre of the University of Surrey has performed a series of wind tunnel experiments where concentration fluctuations have been measured. These experiments refer to the dispersion of a passive gas in a street canyon between 4 identical rectangular buildings under different wind directions. High frequency concentrations have been measured in several positions in the street canyon and concentration fluctuations data have been derived.

These experiments have been selected for computational simulation because they are adequately documented; they include a large number of both concentration and concentration fluctuation measurements, thus favouring the statistical examination of the results; they represent a real-life situation of pollutant dispersion in the cross-junction of two street canyons, while retaining some geometric simplicity.

The geometrical configuration of the wind tunnel experiments consisted of an array of four identical, symmetrically placed boxes, forming a street canyon junction of width 120 mm. Each box was 500 mm



Figure 1 Geometrical configuration of the case.

 $\times$  700 mm  $\times$  125 mm. Several incident wind directions were tested during the experiments. For the simulations in this paper the incident wind direction of 15° relative to the shorter street canyon central line has been selected (Figure 1).

The wind tunnel inflow conditions simulated a neutral atmospheric boundary layer flow with a free-stream velocity of 2 m/s. The pollutant source was a point source placed at several positions along the centre-lines of the two street canyons. For the simulations performed in this paper the selected source location was 420 mm upwind of the centre point of the cross-junction. The diameter of the source was 11 mm, at a height of 10 mm above ground and the polluting gas was released in a downward direction at a rate of 5 l/min. The gas was a 3% volumetric mixture of ethane with air, very close to passive from the density point of view.

The measurements that were performed during the experiment used Laser Doppler Anemometer (LDA) for

the velocity, a Slow Flame Ionisation Detector (SFID) gas sampling system for the low frequency concentrations and a Fast Flame Ionisation Detector (FFID) for the high frequency concentrations. From the latter, the concentration fluctuations were also derived. All the concentration measurements represent the steady-state situation.

For the computational simulations presented in this paper the LDA and FFID measurements have been used. The LDA measurements of velocity and turbulence were taken upwind of the buildings area and they have been used for the computational simulation of the neutral boundary layer. The FFID measurements were taken in the street canyon area at several cross sections and at 3 height levels: 20 mm, 60 mm and 110 mm. In total  $102 \times 3 = 306$  measurements of concentration and concentration fluctuations were available. These have been used for the comparison of the results of the computational simulation and the evaluation of the model.

The measured concentrations were subsequently non-dimensionalised using the characteristic physical quantities of the problem: the height of the buildings  $(0.125 \text{ m})$ , the free-stream velocity  $(2 \text{ m/s})$ , the source flow rate (83.3  $\times$  10<sup>-6</sup> m<sup>3</sup>/s), and the source concentration (29700 ppm).

Further details about the wind tunnel experiments can be found in Grigoriadis and Robins (2001).

#### 4 Computational simulation

The simulation domain was rectangular with the x-axis aligned with the short side of the buildings (Figure 1), the y-axis along the long side of the buildings and the z-axis in the vertical direction. The dimensions were 4.90 m for the x-axis, 4 m the y-axis and 1 m in the vertical. The discretisation was 79  $\times$  83  $\times$  34 cells in the x-, y- and z-axis respectively.

The computational simulation of the experiment was performed using the code ADREA-HF, in 2 steps. The first step was the simulation of the oncoming boundary layer. This was achieved by solving the one dimensional momentum equation in the vertical direction and by adjusting the "driving force" of the pressure gradient to obtain the vertical profiles of velocity and turbulent kinetic energy in agreement with the measurements. The second step consisted of performing the full three-dimensional flow and dispersion calculations, using as initial and boundary conditions the profiles obtained from the first step. The run ended when a steady-state situation was achieved.

The evaluation of the model results consisted of comparing them to the observations. The calculated three-dimensional fields of concentration and concentration fluctuations were interpolated to obtain the values at the exact locations of the FFID measurements. Then the calculated values were plotted against the measured ones as "scatter-plots" (Figures 2 and 3). It can be seen from these figures that the large majority of the points lies in the area delimited by the factor-of-two lines. The model tends to overestimate some concentrations and fluctuations at the lowest level of 20 mm. Another way of comparing is by plotting contours of concentration and concentration fluctuations at the three horizontal levels, where the measurements were taken. This is possible because the FFID measurements where taken at an adequately fine grid. The comparison of the calculated and measured contours for the level at 20 mm is given in Figure 4 for the concentration and in Figure 5 for the fluctuations. It can be observed that for this level the area where the model overestimates the concentrations and fluctuations lies immediately downwind of the source.



**Experimental** 

 $\Omega$ 

0 100

Figure 2 Calculated vs. experimental concentrations.





 Experimental (left) and calculated (right) concentrations contours at the horizontal level of 20 mm.



Figure 5 Experimental (left) and calculated (right) concentration fluctuations at the level of 20 mm.

#### 5 Conclusions

Computational simulation of a wind tunnel experiment is presented in this paper. The case refers to the dispersion of a passive gas in the cross-junction of two street canyons, formed by an array of four identical rectangular buildings. The simulation aims at the evaluation of a model for concentration fluctuations. Model results and observations for concentrations and concentration fluctuations are compared, in the form of scatter and contour plots. The agreement is quite satisfactory and the majority of values lie in the factor-of-two range. There is a tendency of model overestimation at the lowest level of the measurements in the area immediately downwind of the source.

#### **References**

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