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E.A. AUTHOR1[1], and C.E. AUTHOR2[2] (***Author name(s):*** Arial 11 pt, Bold, caps, centered, "and" before last name - Corresponding author: underlined)

[1] Organization and Department Name of Author1, [2] Organization and Department Name of Author2 (Arial 11 pt, centered, full postal address. E-mail address of corresponding author)
e-mail: xxx@xxx.xx

EXTENDED ABSTRACT

The effect of the photochemical cycle on the NO_2 concentration within a typical square (B/H=1) street canyon is studied. For this purpose the microscale model MIMO is applied based on wind tunnel experimental data in order to validate it and to identify the wind velocity filed established for such a geometrical configuration. The chemical module is subsequently applied and first results for night-time chemistry indicate clearly an important increase in the NO_2 concentrations along the street canyon.

The mathematical model..... (***Extended abstract:*** till the end of 1st page (approx. 400 words), Arial 11 pt, fully justified.).....
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1. INTRODUCTION

In the past decades, one of the issues that have attracted increased attention is the degradation of air quality in urban, and therefore, densely populated areas. The aggregation of human activities, especially in these areas of insufficient ventilation, recurrently leads to pollutant concentration levels much higher than the limits set by the World Health Organisation, the EU or the local government. The dispersion of pollutants in urban environments is dominated by the wind flow around complex building structures. Down-wash phenomena and increased local turbulence strongly influence not only the mean flow field but also the diffusion parameters. A typical configuration is the so-called street canyon, formed along a street in a densely built urban area. At the bottom of a street canyon, the vehicles emit gaseous pollutants in the form of buoyant plumes. Under certain conditions, e.g. for non-zero wind component perpendicular to the street, higher concentration levels are observed on the leeward than on the windward side of the street canyon. Due to their rather coarse resolution mesoscale models can not predict those influences accurately. Furthermore, chemical reactions with small time-scales, which take place in the street canyon area immediately after emission, can have a decisive effect on the composition of the pollutants before scales are reached which are comparable to the resolution of mesoscale models.

Microscale models take explicitly into account building structure and are able to predict wind fields and dispersion of pollutants within urban areas and can, therefore, indicate areas of high pollutant concentration in the vicinity of buildings. Moreover, microscale models, taking into account such chemical processes as NO-NO_2-O_3 fast cycles, can provide mesoscale models with more accurate emission data.

Atmospheric flow and pollutant dispersion over urban areas are affected by phenomena belonging to different scales. Regional transport and the flow in the upper part of the planetary boundary layer are mainly determined by mesoscale phenomena. Flow, turbulence and pollutant dispersion near the surface are, however, decisively influenced by single or clusters of obstacles such as buildings or street canyons. Hence, multiscale model systems are being developed, starting at local-to-regional scale and going down to the microscale. An example of such a model system is ZEUS, which is currently under development at the Aristotle University of Thessaloniki, based on the mesoscale model MEMO (Flassak, 1990) and the microscale model MIMO. The incentive behind ZEUS is that each scale provides the next smaller one with appropriate lateral boundary conditions for momentum, heat flux and pollutant concentrations. Microscale parametric computations provide improved momentum, heat and pollutant vertical fluxes as input to the larger scales.

Within that frame, the microscale model MIMO (Ehrhard *et al.*, 2000) was selected and validated against wind tunnel experimental data from a two-dimensional multiple cavity case. Subsequently a fast chemistry module was implemented in order to study the effects of such chemical reactions on the NO_2 concentrations, as this pollutant is harmful to human health.

2. MICROSCALE MODEL DESCRIPTION

The microscale model MIMO is a three-dimensional model for simulating microscale wind flow and dispersion of pollutants in built-up areas. It solves the Reynolds averaged conservation equations for mass, momentum, energy and other scalar quantities such as the humidity or the concentration of pollutants. The conservation equation of mass is formulated in terms of the pressure, yielding an elliptic differential equation. The discrete

form of the elliptic equation is solved using a preconditioned conjugate gradient (CG) method. In order to solve for the averaged conservation equations it is necessary to model the unknown Reynolds stresses, which arise from the averaging of the non-linear transport equations, with the aid of turbulence models. The most common turbulence models are based on the eddy viscosity hypothesis by Boussinesq. Depending on the desired accuracy and effort several turbulence models can be applied by MIMO. The standard k- two-equation turbulence model is used for this particular study. For the numerical treatment of advective transport a three-dimensional second-order flux-corrected transport scheme (FCT) is applied. Within MIMO a finite volume discretisation procedure is adopted for solving the governing equations on a staggered grid arrangement. Coordinate transformation is applied to allow non-equidistant mesh size in all three dimensions in order to achieve a high resolution near the ground and near obstacles. In the model MIMO two different possibilities for the initialisation are included. The first possibility is to couple the microscale model MIMO with the mesoscale model MEMO. Alternatively the initial wind field can be calculated from measured data or by applying the power law.

3. CALCULATIONS PERFORMED

3.1. Case specifications and boundary conditions

The case considered in this contribution has been studied experimentally (Rafailidis and Schatzmann, 1995; 1997) In these experiments, wind tunnel models, corresponding to multiple street-canyon configurations with a variety of canyon aspect (street width B to building height H) ratios and roof shapes, were placed in a simulated deep urban boundary layer (see Figure 1). Between two of the buildings, a steady line source S extending across the tunnel was placed. Concentrations were measured at various locations of the neighbouring walls. The wind was orthogonal to the direction of the street and there were buildings at regular intervals both upstream and downstream of the street containing the source in order to simulate an urban roughness. Tests were performed with B/H=1 and with B/H=1/2. In each case measurements of the concentrations were made in the symmetry plane of the set-up using a Laser light sheet visualisation method, with different combinations of roofs neighbouring the street containing the source.
The concentrations were made non-dimensional by utilising the following formula: K=CULH/Q, where C [vol/vol] denotes the tracer concentration, U [m s^{-1}] is the free stream velocity (5 m s^{-1}), H [m] is the building height, L [m] is the length of the line source and Q [vol/s] the source strength. The initial wind field was calculated from velocity and turbulence intensity profiles that were measured along vertical lines over the roofs at several locations. The computational domain consists of five street canyons. At the main inflow boundary, the profiles of the horizontal velocity u, the turbulent kinetic energy k and the rate of dissipation are specified, such as to match the corresponding experimental conditions, while zero values are assigned to the vertical wind velocity v and the concentration C. At the outflow boundary, the gradients with respect to the streamwise direction are set to zero. At solid walls the no-slip condition is applied. The free-stream horizontal boundary is placed at a distance of 7H over the flat building roofs.

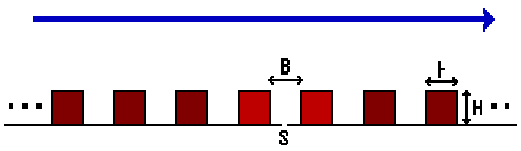

Figure 1: Illustration of the two-dimensional experimental set up.

3.2. Fast chemistry

It has been suggested by other researchers (Palmgren, 1996) that transport and dispersion processes are not the only factors determining source-receptor relationships in urban areas. Chemistry plays an important role in the transformation of pollutants, resulting in degradation of some species and formation of others. Especially inside street canyons where due to the very short distances between sources and receptors and the relatively short residence times of the emitted pollutants, only the fastest chemical reactions can have a decisive effect on the transformation processes of the air mass. Of these fast chemical reactions the photochemical cycle, $NO\text{-}NO_2\text{-}O_3$, is of particular interest as it leads to increase of the NO_2 concentration, a pollutant which is considered to be harmful to human health.
A module for the coupled treatment of fast chemical reactions within street canyons has been developed based on the $NO\text{-}NO_2\text{-}O_3$ cycle:

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Where k ($ppb^{-1}\ s^{-1}$) and j (s^{-1}) are the reaction rate constants for the oxidation of NO and the photolysis frequency of NO_2 respectively.
A semi-implicit treatment scheme of source terms due to chemical transformations is implemented. A source term linearisation was performed in order to calculate the increase or decrease of each chemical's concentration, where:

$$\mathrm{d}[\mathrm{NO}] = \{-k[\mathrm{NO}][O_3] + j[\mathrm{NO_2}]\}dt$$
$$\mathrm{d}[\mathrm{NO}] = \{k[\mathrm{NO}][O_3] - j[\mathrm{NO_2}]\}dt$$
$$\mathrm{d}[\mathrm{O_3}] = \{-k[\mathrm{NO}][O_3] + j[\mathrm{NO_2}]\}dt$$

These equations are then embodied to the transport equations, as source terms due to chemistry, using a simple integration rule.
Different background values for O_3 are assumed while no background values for NO and NO_2 are provided. NO and NO_2 sources at street level are used in order to simulate heavy NOx traffic emissions. In this contribution only night-time reactions were considered, where the reaction rate constant of NO_2 was set to zero.
Work already completed with CFX-TASCflow for night-time conditions allowed quantifying the O_3 depletion and the significant increase of the NO_2 concentration due to oxidation of NO with O_3.

4. RESULTS

4.1. Comparison with experimental data

The case studied for the purposes of this contribution was the square canyon (B/H =1), due to the simplicity of the flow filed evolved which would subsequently be used for the application of the fast chemistry module. Furthermore MIMO should be validated against experimental data.
Figure 2 illustrates the velocity field, as computed by MIMO for the square street canyon case. A primary vortex is established, which results in a wind direction close to the bottom of the street, from the windward to the leeward wall. Moreover, higher wind velocities are observed in the vicinity of the canyon floor and top whereas, towards the centre of the canyon and the vortex formed, velocities drop to almost zero at the centre. Figure 3 shows the comparison between measured and computed non-dimensional

concentrations for the square canyon. In this case the maximum concentrations appear on the leeward wall (marked as A in figure 3), due to the action of the primary vortex, however peak concentrations are slightly under estimated by MIMO. The agreement between computed and measured concentrations is good. Further work has been performed with MIMO in order to study the effects of altering the street canyon geometry on the wind filed and the dispersion of pollutants (Assimakopoulos *et al.*, 2000).

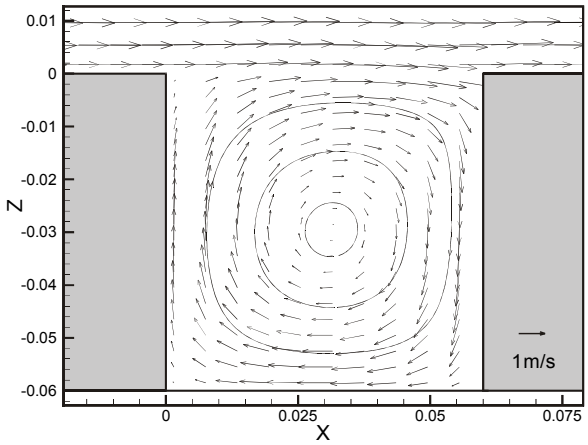

Figure 2: Velocity field as computed by MIMO for the square canyon case.

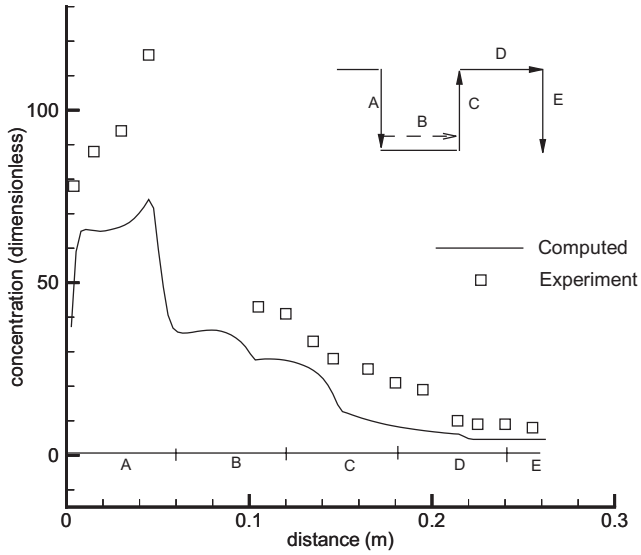

Figure 3: Comparison between measured and computed non-dimensional concentrations for the square canyon case.

4.2. Fast chemistry calculations

The same case specifications and boundary conditions were adopted for the fast chemistry calculations. The NO_x emission rate was assumed to be 1250 μg m^{-3}sec and O_3 concentrations ranged from 30 ppb to 70 ppb. The ratio of NO_2/NO_x was set to 5% following the suggestions of other researchers. In figures 4,5 and 6 the effect of the chemical reactions taking place immediately after emission is clearly seen for the leeward wall, the centre of the cavity and the windward wall respectively.

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5. CONCLUSIONS

The microscale model MIMO was validated against wind tunnel experimental data. Having established its satisfactory performance a fast chemistry module was created and embodied with MIMO in order to study the effects on the concentration of NO_2. It was found that for night-time conditions with a steady background O_3 concentration NO_2 rises. The relationship between the NO_2/NO_x ratio is almost linear and it rises with higher background O_3 concentration. Furthermore, it was found that the ratio varies along the canyon rising dramatically from the leeward wall to the windward wall, whereas maximum NO_x concentrations are met at the leeward wall. Further work will be performed in order to study daytime chemical reactions and their effect on NO_2 concentrations within street canyons.

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