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(include a fax number and e-mail address). Full postal addresses must be given for all co-authors.

All manuscripts should be carefully edited to eliminate redundancy. All abbreviated terms should be explained on first occurrence.

Manuscripts should begin with an Abstract of up to 200 words that contains concise factual information on objectives, methods, results, and conclusions.

Opinions, obscure terms, and jargon should be avoided. Key Word Index should follow, including a maximum of 10 Keywords. Avoid words that are referred in title. The body of the text should begin with a statement of the objectives of the work. It should include citations of published related work and sections on Methods, Results, Discussion and Conclusions of the study. An Acknowledgement section may follow the Conclusions.

The paper should be up to 10 pages long, including diagrams, references and tables.

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References should be given as in the following examples, for books, articles in journals, papers in contributed volume or proceedings of conferences and reports:

- Sawyer C.N., McCarty P.L. and Parkin G.F. (1994), *Chemistry for Environmental Engineering*, Fourth Edition, McGraw Hill, New York.
- Lekkas, T. and Gosh, C.D. (1996a), Treatment of hazardous waste, *Global NEST Journal*, **2**, 98-121.
- Bennarie, M.M. (1982), Air pollution modeling operations and their limits, In: *Mathematical Models for Planning and Controlling Quality*, Fronza, G. and Melli, P. (eds.), Pergamon Press, UK.
- Lekkas, T. and Gosh, C.D. (1996b), Survey of hazardous waste sources, Rep. No. 12345, U.S. EPA, Washington D.C.

Only written papers that have been published in the literature should be referenced. If necessary to reference an unpublished work, follow the example given:

- Rajasekar, A. (1989), Semantics for logic programs. Ph.D. Thesis, Department of Computed Science, University of Maryland.

For online citations (web sites) date of access should be included.

**7. Manuscript Length:** Manuscripts for Research Papers should be no more than 10 single-spaced (Arial 11 point) pages in length (8 pages for Research Notes and Technical Papers) and should follow the general format for Research Papers. Discussions of Research Papers and Research Notes should be no more than 2 single-spaced pages in length, including tables and figures, which should be kept to a minimum.

**8. Tables and Figures:** Tabular or graphical data should be adequately discussed in the text. In particular, similar data should not be presented in both figures and tables. Tables are to be concise and contain only the information essential to the text. Columns containing few entries or full columns of data that vary only slightly should be avoided. Judicious use of table footnotes can greatly simplify the presentation.

Graphs should be used to support correlations or illustrate points made in the text, not merely to present data. Legends identifying curves should be contained within the graphs, not in the captions. Graphs and line drawings should be drawn carefully and must be large enough for clarity. All graphs and figures should be of sufficient quality to ensure that they are legible when printed (at least 300 dpi). Dot matrix or impact computer printouts using fabric ribbons

or tracings are unacceptable. Figures and tables should be incorporated into the main body of the text.

**9. Units:** All data in the text, figures and tables must be reported in metric notation and International System of Units (SI) nomenclature. Conversion of any non-metric data will be requested from the author before publication. Use negative indices rather than / and leave space between symbols, e.g.  $\text{m s}^{-1}$  not  $\text{ms}^{-1}$  or  $\text{m/s}$ .

**10. Equations:** Equations and formulas should be numbered separately and sequentially throughout the text. All variables and special symbols, such as Greek letters, must be clearly identified and explained, including units when appropriate.

**11. Photographs:** Submission of photographs should be limited to those essential to an adequate understanding of the text. When necessary, photographs should be sharp, glossy, prints identified on the back with a felt-tip pen. Photographs will not be published in color within an issue except in rare circumstances and at the discretion of the Executive Editor.

**12. Nomenclature** should conform to that most frequently used in the science and engineering field concerned.

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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<sub>2</sub>-O<sub>3</sub> 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<sub>2</sub> concentrations, as this pollutant is harmful to human health.

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## **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- $\epsilon$  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.

**CALCULATIONS PERFORMED**

**Case specifications and boundary conditions**

The case considered in this contribution has been studied experimentally (Rafailidis Schatzmann, 1995). 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  $\epsilon$  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.

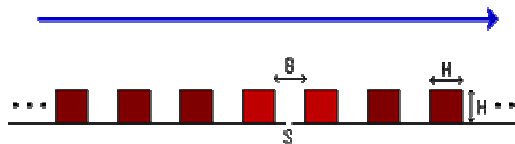


Figure 1. Illustration of the two-dimensional experimental set up.

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**Fast chemistry**

It has been suggested by other researchers (Palmgren *et al.*, 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-NO<sub>2</sub>-O<sub>3</sub>, is of particular interest as it leads to increase of the NO<sub>2</sub> 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-NO<sub>2</sub>-O<sub>3</sub> cycle:

Table 1. xxxxxxxxxxxxxxxx xxxxxxxxxxxx xxxxxxxxxxxx.....


Where  $k$  ( $\text{ppb}^{-1} \text{s}^{-1}$ ) and  $j$  ( $\text{s}^{-1}$ ) are the reaction rate constants for the oxidation of NO and the photolysis frequency of  $\text{NO}_2$  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:

$$\begin{aligned} d[\text{NO}] &= \{-k[\text{NO}][\text{O}_3] + j[\text{NO}_2]\}dt \\ d[\text{NO}_2] &= \{k[\text{NO}][\text{O}_3] - j[\text{NO}_2]\}dt \\ d[\text{O}_3] &= \{-k[\text{NO}][\text{O}_3] + j[\text{NO}_2]\}dt \end{aligned}$$

These equations are then embodied to the transport equations, as source terms due to chemistry, using a simple integration rule.

Different background values for  $\text{O}_3$  are assumed while no background values for NO and  $\text{NO}_2$  are provided. NO and  $\text{NO}_2$  sources at street level are used in order to simulate heavy  $\text{NO}_x$  traffic emissions. In this contribution only night-time reactions were considered, where the reaction rate constant of  $\text{NO}_2$  was set to zero.

Work already completed with CFX-TASCflow for night-time conditions allowed quantifying the  $\text{O}_3$  depletion and the significant increase of the  $\text{NO}_2$  concentration due to oxidation of NO with  $\text{O}_3$ .

## RESULTS

### 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 field 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.

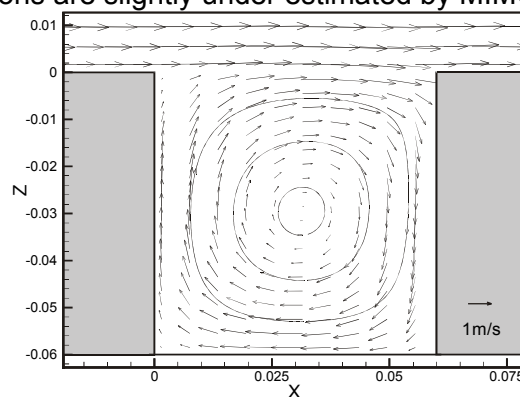


Figure 2. Velocity field as computed by MIMO for the square canyon case.



raises. The relationship between the NO<sub>2</sub>/NO<sub>x</sub> ratio is almost linear and it rises with higher background O<sub>3</sub> 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<sub>x</sub> concentrations are met at the leeward wall. Further work will be performed in order to study daytime chemical reactions and their effect on NO<sub>2</sub> concentrations within street canyons.

## REFERENCES

References:  
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