The obstacle resolving microscale model MITRAS

A contribution to subproject SATURN

K. Heinke Schlünzen, G. Bischof, O. Knoth[1], M. Lambrecht[1], B. Leitl, S. Lopez[2], C. Lüpkes[2], H. Panskus, E. Renner[1], M. Schatzmann, T. Schoenemeyer[3], S. Trepte[3], R. Wolke[1],

Meterological Institute, University of Hamburg, Bundesstr. 55, 20146 Hamburg, Germany

Summary

An updated version of the obstacle resolving microscale model MITRAS has been developed. Several modules of the model (turbulence parameterization, chemistry, soot transport, solvers) have been updated, tested stand-alone and are now tested in the framework of MITRAS. For comparison with model results wind tunnel measurements are available. An evaluation scheme for microscale obstacle resolving models has been finalised.

Aim of the research

This SATURN contribution aims to develop an obstacle resolving microscale model (MITRAS, Panskus et al.; 1997; Lambrecht et al., 1998) which can be used to simulate atmospheric flow and pollutant transport in an area of several hundreds to some thousands of metres with a horizontal resolution of some metres. MITRAS includes passive tracer transport as well as chemical reactions by directly solving the gas phase chemistry within the micro-scale model. The chemistry module considers all important chemical reactions close to traffic sources. Soot is transported as aerosol with its deposition dependent on size. Soot is treated as a sink for VOC compounds. For a realistic simulation of mixing effects a turbulence parameterization for obstacle resolving models has been developed. To evaluate the model performance an evaluation strategy was introduced which is using wind tunnel data as well as field measurements. MITRAS is prepared to be nested in urban scale models by application of the nudging technique.

The MITRAS development is a result of a co-operation of the Alfred Wegener Institute for Polar and Marine Research, Bremerhaven, the Fraunhofer Institute for Atmospheric and Environmental Research, Garmisch-Partenkirchen, the Institute for Tropospheric Research, Leipzig, and the Meteorological Institute, University of Hamburg.

Activities during the year

The modules of the updated model (turbulence parameterization, chemistry, soot transport, solvers) have been tested separately first. Currently the modules are tested in the framework of the MITRAS model. An evaluation concept for obstacle resolving microscale models has been developed and tested (Panskus, Schlünzen, 2000; Panskus, 2000). The updated version of MITRAS includes an K-ε-turbulence closure scheme (SATURN activity 19), an improved numerical solver (SATURN activity 6) and an on-line calculation of chemistry (SATURN activity 27). In addition, a module for calculation of shading effects by buildings was implemented in MITRAS. The gasphase chemistry was enhanced by heterogeneous reactions (SATURN activity 27). The complete model MITRAS containing all new modules is now tested by using the new evaluation concept which is applicable to urban transport and flow models (SATURN activity 29; Panskus, Schlünzen, 2000). All validation data have been

[1] Institut für Tropospärenforschung, Leipzig, Germany
[2] Alfred Wegener Institut für Polar und Meeresforschung, Bremerhaven, Germany
[3] Fraunhofer Institut für Atmosphärische Umweltforschung, Garmisch-Partenkirchen, Germany

compiled from wind tunnel measurements (SATURN activity 67, Figure 1; http://www.mi.uni-hamburg.de/cedval/).

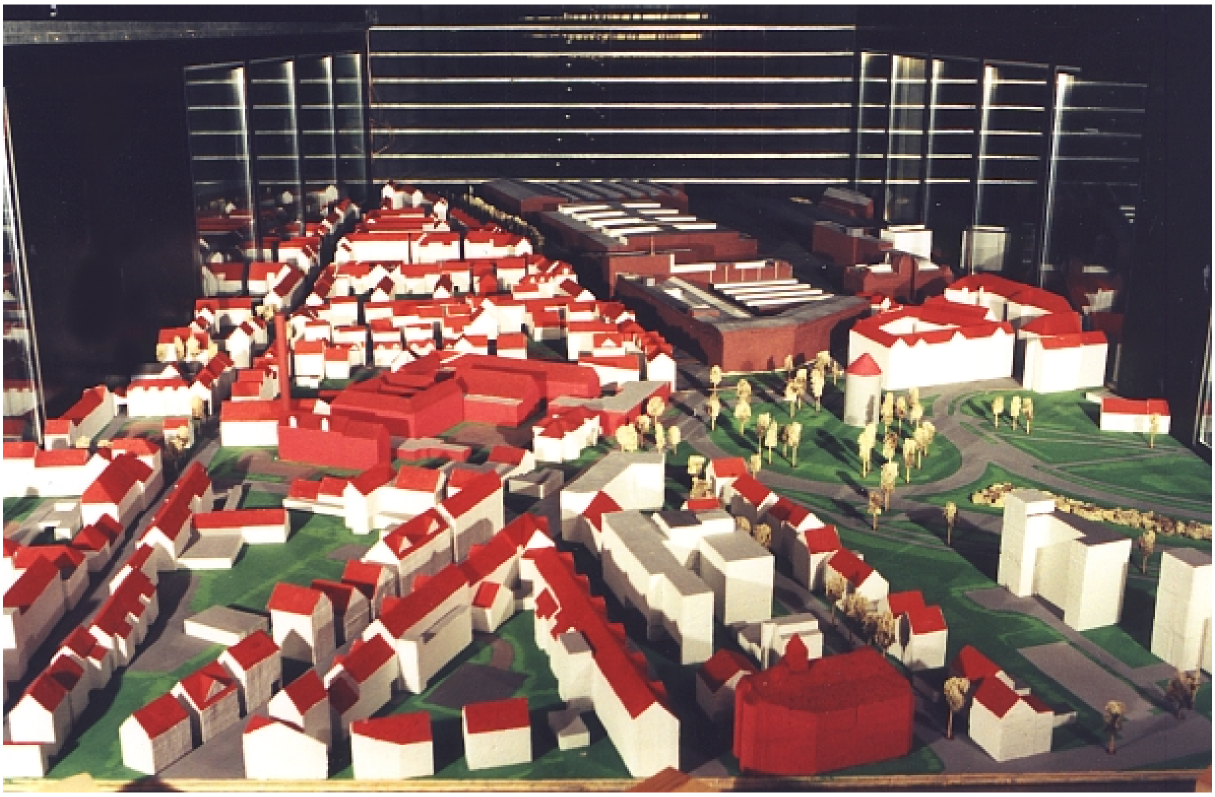

Figure 1: Wind tunnel model for the "Göttinger Straße" in Hannover.

Principal results

Different turbulence parameterizations have been tested in MITRAS. It could be shown by comparison with wind tunnel data that the standard K-ε-turbulence closure overestimates the production of turbulent kinetic energy K at stagnation points at the windward side of buildings. A reformulated K-ε-closure by Kato and Launder (1993) was applied in which the original production term given by the square of the strain rate is replaced by the product of this strain rate and a rotation parameter. It can be seen from Figure 2 that near the stagnation point in front of the building the production of turbulent kinetic energy is now more realistic. Further apart from the obstacle the flow is independent of the applied turbulence closure. Furthermore, an K-ε closure of Murakami (Tsuchiya et al., 1997) was implemented in which the eddy diffusivity depends on the relation of strain rate and a rotation parameter. It has been shown by comparison of MITRAS results with field observations that this closure gives the best results (Garbrecht et al., 1999).

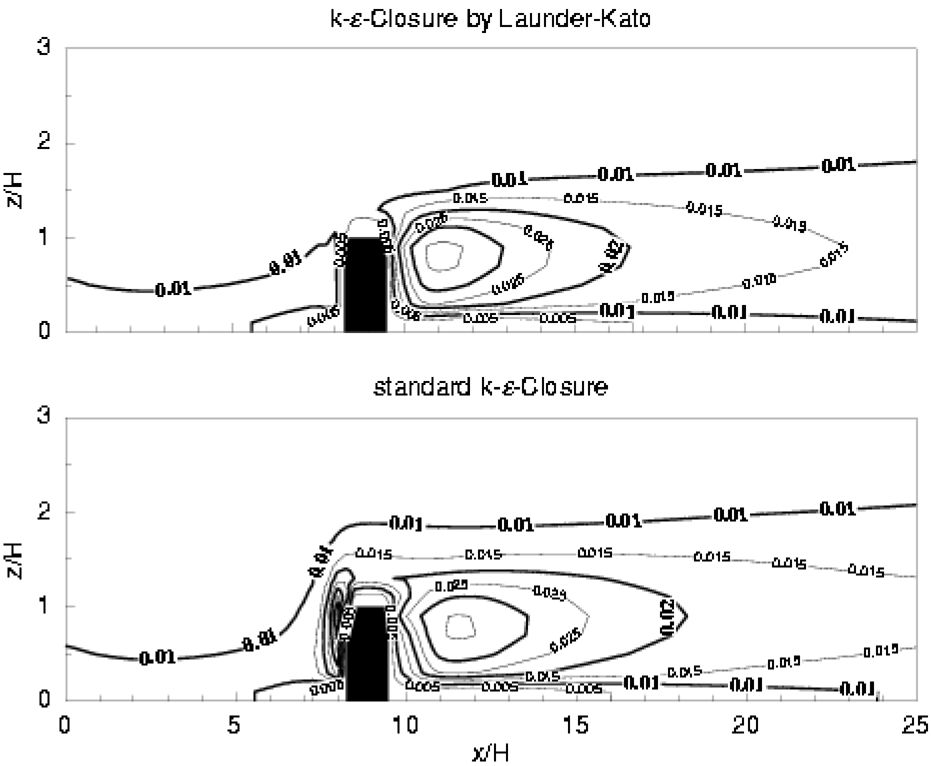

Figure 2: Simulated normalized turbulent kinetic energy (K/u^2) calculated with K-ε-closure of Kato, Launder (top) or with the standard K-ε-closure (bottom).

The microscale model MITRAS has been coupled with the chemical transport model MUSCAT (**Mu**lti**S**cale **C**hemistry **A**erosol **T**ransport; Knoth and Wolke, 1998) and applied in an online mode. The model MADMAcS (Wilck and Stratmann, 1996) has been included in MUSCAT to describe aerosol dynamical processes. Particle size distribution and aerosol dynamical processes are simulated using the modal technique, where the mass fractions of all particles within one mode are assumed to be identical. In the first microscale applications, transport has been considered as well as coagulation, deposition, and sedimentation.

Some simulation results for a soot particle distribution in a street canyon are given in the Figures 3-5. 80x80x24 grid points and a horizontal grid size of 5m were used. The simulation is performed with three modes (nucleation, accumulation and coarse mode) and two kinds of particulate matter (soot and background aerosol). Soot is emitted from a line source in the nucleation mode only.

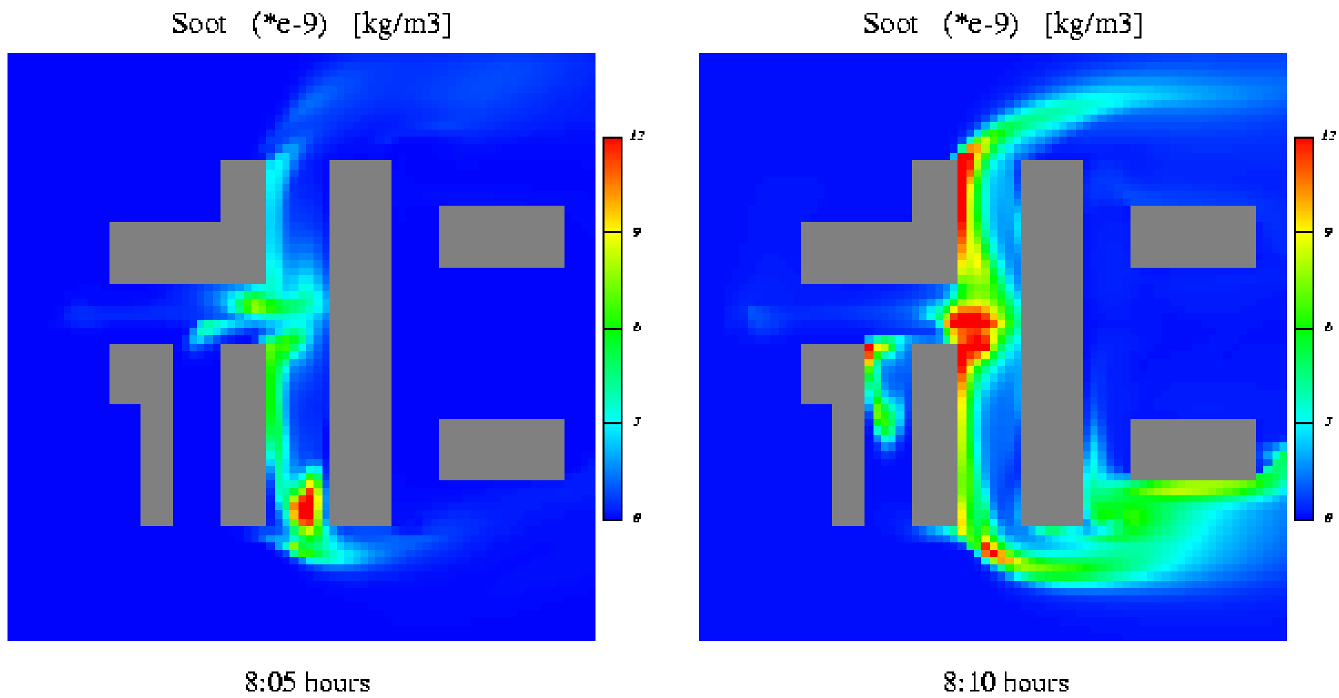

Figure 3. Mass concentration of soot after 5 minutes simulation time (left) and after 10 minutes simulation time (right).

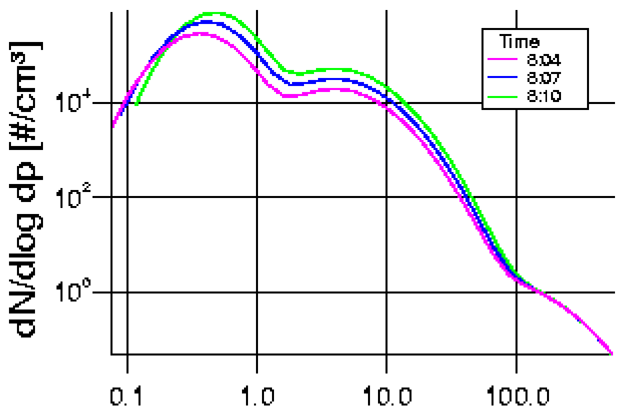

Figure 4. Number distribution of particles at a grid point in lee of the street canyon.

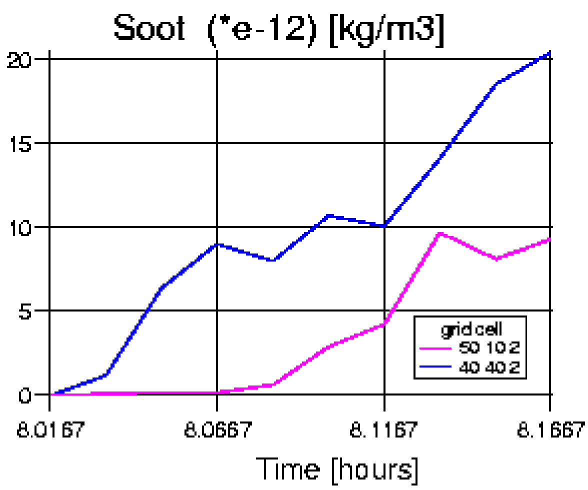

Figure 5. Mass concentration of soot in the accumulation mode at two grid points in lee of the street canyon for different simulation times.

Shading by buildings leads to a significant change of temperature- and flow field in a street canyon and can reduce the photolysis rates by a factor of 2 in the shaded areas. In consequence the calculated three-dimensional distribution of secondary pollutants with the improved MITRAS is different from the version without consideration of building effects. In Figure 6 the impact of shading on the NO_2 concentration in a street canyon is presented. In one case, the left-hand side of the street canyon is shadowed, in the other case, the right-hand side of the street canyon is shadowed. It is obvious, that the NO_2-concentration increases significantly in the left-hand side of the street canyon if the left-hand side of the street canyon is exposed to the sun.

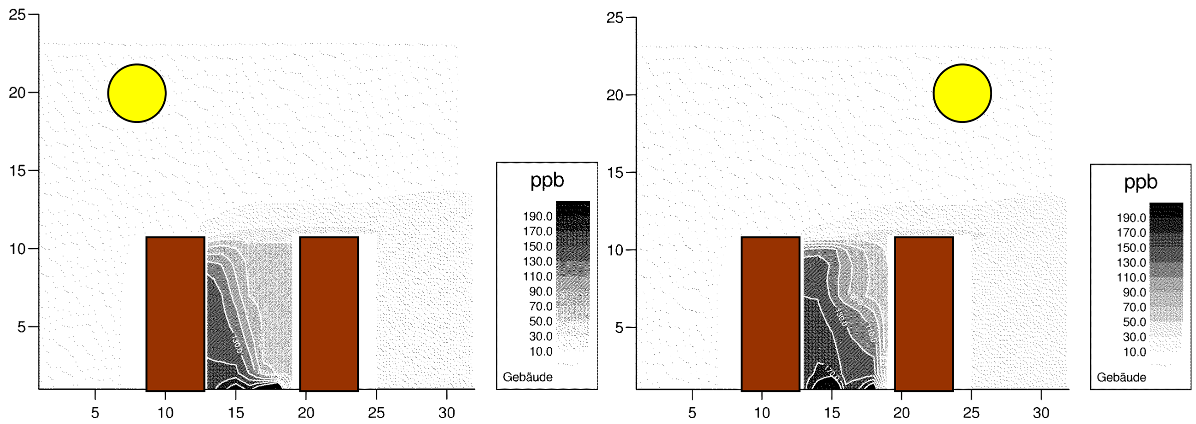

Figure 6: Vertical cross section of NO_2-concentration within a street canyon calculated with MITRAS including shading effects.

Based on sensitivity studies for the heterogeneous reactions

$$HNO_3 \xrightarrow{carbon} NO_2$$
$$HNO_3 \xrightarrow{carbonf} NO$$
$$NO_2 \xrightarrow{carbon} NO$$
$$O_3 \xrightarrow{carbon} O_2$$

the effect of diesel particles on gasphase concentrations is considered in MITRAS. From the results of Lary et al. (1997) it follows that the direct loss of ozone is negligible. In contrast, the other reactions are important and have to be considered in street canyons. In the consequence these reactions lead to a decrease of photooxidant concentration. In some of the simulations it turned out, that consideration of the first three reactions leads to a decrease of ozone by 80%.

The evaluation concept for obstacle resolving numerical models (SATURN activity 29) was successfully tested with a previous version of MITRAS, which used a Prandtl-Kolmogorov turbulence closure and neglected wall functions at the building surfaces. The evaluation helps to detect model shortcomings. In Fig. 7 model results for the flow around a cube are shown for calculations with and without wall functions. In the lower panel the wind tunnel measurements are given. As expected the agreement between measured data and model results is better in the simulation which applies wall functions.

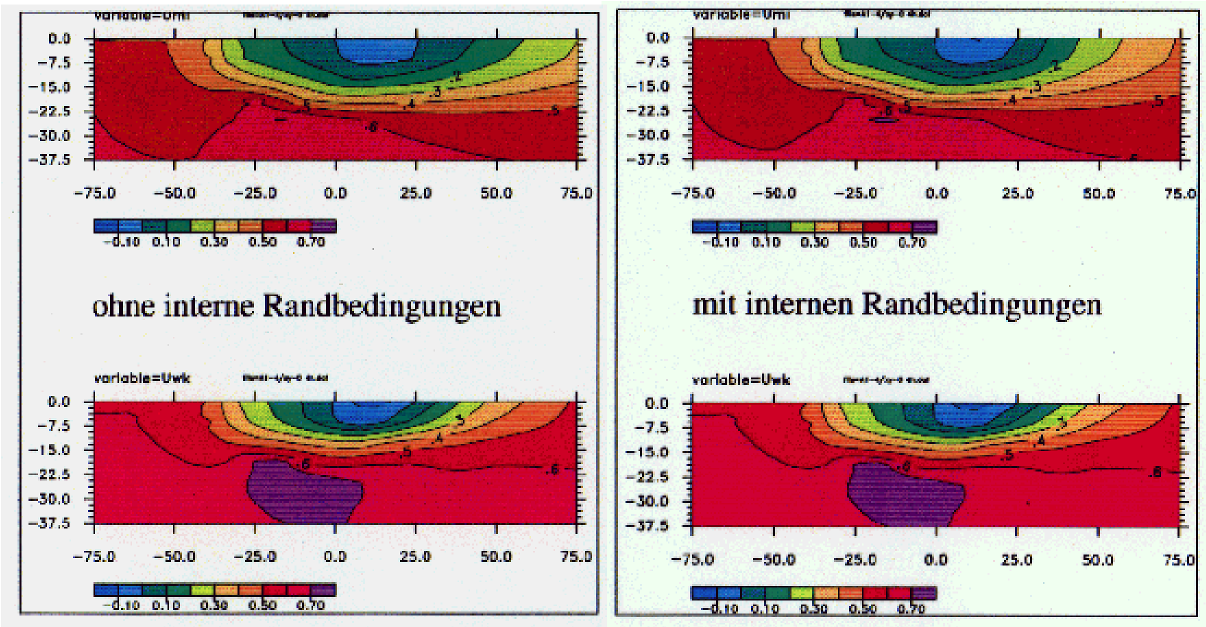

Figure 7: Horizontal cross section at 0.4H for the u-component of the velocity around a cube in neutrally stratified boundary layer. On the lower panel wind tunnel measurements are given. On the upper panel model results without wall functions (left) and including wall functions (right) are shown.

Main conclusions

The modules of the updated model have been tested as stand-alone modules and within the framework of an older version of MITRAS. The reformulated E-ε-closure turns out to be important in order to calculate proper fluxes close to buildings. Shading effects by buildings and heterogeneous reactions need to be considered. Gas phase chemistry and soot transport strongly depend on the local wind field due to the heterogeneity of the mixing.

The updated model, the data sets for evaluation and the evaluation concept developed can be applied for simulating flow phenomena within the obstacle layer and for the evaluation of obstacle resolving models. Using the MITRAS model system, the influence of a detailed description of small scale aerosol processes in urban areas on the net emission and deposition of species and aerosols in the larger scale can be investigated.

Aim for the coming year

The tested modules are all included in MITRAS already. The updated version of MITRAS needs to be tested by applying the new evaluation concept. A documentation of the complete model will be prepared. A user manual will help non-experts to use the model, a detailed model description and user guide will help experts to change the program code.

The tested version of MITRAS will be applied to a field site in Hannover (Göttinger Straße). Model results will be compared with wind tunnel data and field measurements

Acknowledgements

This work was funded by the German Minister of Education and Research within the German Tropospheric Research Initiative under grant number 07TFS10. The authors are responsible for the contents of this publication.

References

Garbrecht, T., C. Lüpkes, E. Augstein and C. Wamser; Influence of a sea ice ridge on low level airflow, *J. Geophys. Res*.,. **104 D20** (1999) 24499-24507.

Kato, M. and B.E. Launder; The modeling of turbulent flow around stationary and vibrating square cylinders, *9th symposium on tubulent shear flows, Kyoto*, (1992) 10-4-1 - 10-4-6.

Knoth, O. and R. Wolke; An explicit-implicit numerical approach for atmospheric chemistry-transport modelling, *Atmos. Env*. **32** (1998) 1785-1797.

Lambrecht, M., O. Knoth and E. Renner; Development of numerical schemes for high-resolution urban scale models, *Proc. EUROTRAC Symposium'98*. Editors: P.M. Borrell and P. Borrell. WITPress, Southampton. (1999).

Lary, D.J., A.M. Lee, R. Toumi, M.J. Newchurch, M. Pirre and J.B.; Renard: carbon aerosols and atmospheric photochemistry, *J. Geophys. Res.* **102** (1997) 3671-3682.

Panskus, H.; Vorschrift zur Evaluation hinernisauflösender mikroskaliger Modelle und ihre Anwendung auf das Modell MITRAS; *PhD thesis Fachbereich Geowissenschaften*, Universität Hamburg (2000) 103.

Panskus, H., O. Knoth, M. Lambrecht, C. Lüpkes, M. Schatzmann, K.H. Schlünzen, T. Schönemeyer and S. Trepte; Konzeption eines mikroskaligen Modells in bodenfolgenden Koordinaten mit Chemie, *Proc. Fachtagung METTOOLS III*, Universität Freiburg (1997).

Panskus H. and K.H. Schlünzen; An Evaluation strategy for prognostic micro-scale numerical models of the obstacle layer, *Env. Monitoring and Assessment*, submitted. (2000):

Wilck, M. and F. Stratmann; A lognormal model for the size-resolved treatment of particle dynamics and liquid phase chemistry, *J.Aerosol Sci.* **27** (1996) 583-584**.**

Tsuchiya, M., S.Murakami, A. Mochida, K.Kondo and Y.Isjida; Development of a new K-ε-model for flow and pressure fields around a bluff body, *J. of Wind Engeneering and Industrial Aerodynamics* **67&68** (1997) 169-182