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A PHOTOCHEMICAL AIR POLLUTION MODEL

T. TURÁNYI, L.HASZPRA*, T. BÉRCES

Central Research Institute for Chemistry
H-1525, P.O.B. 17,Budapest, Hungary

* Institute for Atmospheric Physics
H-1675, P.O B. 39, Budapest, Hungary

SUMMARY

A photochemical air pollution model suitable for urban air quality calculations has been developed and tested under realistic conditions. The model treats pollutant transport by adopting the Langrangian approach. Detailed chemistry is contained in the model which includes emission and deposition processes taken intoaccount as first order steps. A recent version of sensitivity analysis is used to reduce the original reaction mechanism to a favourable size.

KEY WORDS: air pollution, photochemical smog, Langrangian approach, reaction kinetics, sensitivity analysis.

INTRODUCTION

Increasing air pollution is a serious problem all over the world. The great expenditures required in environmental protection demand the development of cost-effective control strategies. Ellaboration of such strategies presumes the understanding of the relation between emission intensities and airborne concentrations under different meteorological conditions. Such informations are provided by air quality models.

PHYSICAL AND METEOROLOGICAL SUBMODEL

Air quality models describe the distribution of pollutants in the atmosphere and their diurnal variation (Seinfeld , 1986). The simulation of the distribution of pollutants require the numerical solution of the atmospheric transport equation. In our model the Langrangian approach was used.

A wind map was generated by a submodel constructed by

L.Nyitrai (Nyitrai, 1986). It takes into account the change of wind caused by the relief as a function of the height of inversion layer. The diurnal variation of the speed and direction of wind and the height of the inversion layer were selected in accordance with meteorological data registered in Budapest.

Nitrogen- oxides, sulphur-dioxide, carbon-monoxide, aliphatic and aromatic hydrocarbons and oxo-compounds are the major primary pollutants in an urban air. In our model communal, industrial and traffic sources of emission are distinguished. Diurnal variation of emission is taken into account. For the spatial resolution of emission a 4 km x 4 km grid was adopted and the emission was regarded homogeneous within each square.

REACTION MECHANISM AND SENSITIVITY ANALYSIS

The chemical submodel describes the consumption of primary pollutants and the formation of secondary products. The emission and deposition are included in the mechanism as first order processes.

In the literature several photochemical mechanisms have been suggested for inclusion in atmospheric models. Our model is based on the mechanism of Atkinson et al (1983). Modifications proposed by Leone et al (1985) are also taken into account.

The most computer-time consuming step in the use of an air quality model is the solution of the chemical kinetic differential equations, therefore any reduction of the mechanism considerably accelerates the run of the model. Mechanism reduction was carried out by rate sensitivity analysis using a recently developed technique (Turányi et al, 1987) that considers the sensitivity of product formation on the effect of the change of parameters. (This technique differs basically from the conventional sensitivity analysis where the effect of parameter change on the concentrations is considered.) The new method was showed to give much detailed sensitivity information required less computer time. The principal component analysis (Vajda et al, 1985) of the rate sensitivity matrix pinpoints the less important or redundant reactions and in addition reveals the connections and relations between important parameters. (The method is appropriate for investigating not only reaction mechanisms, but any models described by differential equations.)

The reduced model was tested against smog chamber experiments (Pitts et al, 1977). The stiff kinetic differential equation system was solved by an implicit, fourth order Runge-Kutta method (Gottwald et al, 1983).

APPLICATION OF THE MODEL.

The utility of the photochemical air pollution model has been tested by calculations made for realistic meteorological and emission conditions In these calculations temperature, humidity, solar light intensity, direction and strength of wind as well as typical composition and intensity of emission of primary pollutants were chosen in accordance with measurements made during the summer months in Budapest and surrounding.

The air pollution model was used to study the effect of some input data (first of all the data characteristic for the wind and emission) on the air quality. The results allowed us to identify the meteorological conditions which may result in serious smog events in Budapest and to reveal the correlations between the composition of the primary pollutants emitted and the air quality. Calculations showed that maximum oxidant concentrations can occur under certain conditions far removed downwind from the polluting source.

Among others, the variation of the formation of especially dangereous secondary pollutants has been studied as a function of meteorological and emission conditions. Thus, the accumulation of nitric acide in the air was calculated (Haszpra et al., 1986).

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REFERENCES

Atkinson R., Lloyd A.C., Winges L. (1982), An updated chemical mechanism for hydrocarbon $/NO_x/SO_2$ photooxidations suitable for inclusion in atmospheric simulation models, Atmos. Environ., 16, 1341-1355.

Gottwald B.A., Wanner G.(1981), A reliable Rosenbrock integrator for stiff differential equations, Computing, 26, 355-360.

Haszpra L., Turányi T. (1986), Production of nitric acid in the atmosphere under different conditions, Időjárás, 90, 332-338.

Leone J. A.,Seinfeld,J.H.(1986)Comparative analysis of chemical reaction mechanisms for photochemical smog, Atmos. Environ., 19, 437-464.

Nyitrai L. (1986) Unpublished results.

Pitts J.N. et al (197'), Mechanisms of photochemical reactions in urban air, U.S. EPA Report, EPA-600/3-79-110

Seinfeld J.H. (1986), Atmospheric chemistry and physics of air pollution, Wiley, New York.

Turányi T., Bérces T., Vajda S. (1987), Local sensitivity analysis: The concept of reaction rate sensitivity and its application in the study of kinetic mechanisms, Int. J. Chem. Kinet., to be published.

Vajda S., Valkó P., Turányi T. (1985), Principal component analysis of kinetic models, Int. J. Chem. Kinet., 17, 55-81.