Advances in Air Pollution Modeling for Environmental Security

Edited by

István Faragó, Krassimir Georgiev
and Ágnes Havasi

NATO Science Series

IV. Earth and Environmental Sciences – Vol. 54

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Advances in Air Pollution Modeling for Environmental Security

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PREFACE

The protection of our environment is one of the major problems in the society. More and more important physical and chemical mechanisms are to be added to the air pollution models. Moreover, new reliable and robust control strategies for keeping the pollution caused by harmful compounds under certain safe levels have to be developed and used in a routine way. Well based and correctly analyzed large mathematical models can successfully be used to solve this task. The use of such models leads to the treatment of huge computational tasks. The efficient solution of such problems requires combined research from specialists working in different fields.

The aim of the NATO Advanced Research Workshop (NATO ARW) entitled "Advances in Air Pollution Modeling for Environmental Security" was to invite specialists from all areas related to large-scale air pollution modeling and to exchange information and plans for future actions towards improving the reliability and the scope of application of the existing air pollution models and tools. This ARW was planned to be an interdisciplinary event, which provided a forum for discussions between physicists, meteorologists, chemists, computer scientists and specialists in numerical analysis about different ways for improving the performance and the quality of the results of different air pollution models.

The NATO ARW was held at Borovetz (Bulgaria), in the period 8-12 June, 2004. The participants were partly outstanding specialists with international reputation, partly very talented young researchers who will once belong to the first category. About 46 delegates from 17 NATO member countries and partner countries actively participated in the workshop. (In addition to the above NATO participants, there were ten further participants, supported by BULAIR.)

The main objectives of this meeting were the following:
(a) improving the abilities of air pollution models to calculate reliable predictions of the pollution levels in a given domain and in real time by using adequate description of the physical and chemical processes,
(b) implementation of advanced numerical methods and algorithms in the models,
(c) efficient utilization of up-to-date computer architectures,

(d) development of mechanisms for studying particles (including here fine and ultra-fine particles), biogenic emissions, etc.
(e) optimization techniques in the study of the pollution levels, etc.

Plans for developing more advanced and more reliable air pollution models were also discussed. The adaptation of the existing and new models to the new generation of computers was one of the major topics of this meeting.

There were 45 plenary talks given. In the first working day we organized a discussion "Running comprehensive air pollution models on different kinds of computers architectures", while on the next day we had a discussion on "Emission control in air pollution problems". On the third day we organized a discussion about "Data assimilation and solving big optimization problems".

We hope that the participants of the meeting have got new motivation to further applications of the existing results with possible cooperation with specialists from different NATO countries. The exchange of the experience and knowledge of the specialists in air pollution modeling, numerical mathematics, optimal control and parallel computing could facilitate very much the further activities on this area. The participants could present their latest results in the area of air pollution modeling and – as long-term benefits – they will do cooperative research towards reducing the trans-boundary transport of air pollution. It is expected that new collaborations between the NATO and Partner countries institutions and new teams for joint research will be established. The exchange of knowledge, ideas and tools for treatment of the air pollution models for environmental security and the optimal control of emissions can be used for an improvement of the existing models and the development of new ones in the near future.

The editors

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The workshop could not have been successful without the active contribution of all participants.

The editors

MATHEMATICAL MODELING OF THE REGIONAL-SCALE VARIABILITY OF GASEOUS SPECIES AND AEROSOLS IN THE ATMOSPHERE

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Abstract: A three-dimensional numerical model of atmospheric hydrodynamics, transport and photochemical transformation of gas-phase pollutants and aerosol dynamics is considered. New particle formation occurs via binary homogeneous nucleation of sulphuric acid and water vapor, proceeding under the conditions of temperature and humidity fluctuations. The kinetic processes are described by multidimensional equations of condensation and coagulation, where the size-distribution function is given explicitly. Wind flow fields and turbulent characteristics are calculated from the mesoscale nonhydrostatic model of atmospheric hydrodynamics over complex topography. A series of numerical experiments are performed aimed at modeling the photochemical air pollution and aerosol dynamics in two specific regions as well as formation of sulfate aerosol particles in the northern hemisphere. A comparison is given for calculated and measured ozone concentration data.

Key words: Atmosphere, photochemical air pollution, aerosol, nucleation, condensation, coagulation, numerical modeling.

1. INTRODUCTION

Sulfate aerosol plays an important role in different regions: free atmosphere, marine boundary layer, Arctic, urban polluted areas, etc. Tropospheric ozone pollution is another problem of primary interest. Resulting from the interaction between nitrogen oxides and volatile organic compounds, this secondary pollutant is a key indicator for photochemical air pollution. For aerosol modeling, photochemical transformation products are

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of primary importance due to the fact that their vapor condensation leads to primary clusters initiating aerosol formation. Then these clusters interact with background atmospheric nuclei.

At present, there are a number of models for photochemical transport (Hass et al., 1993; Stockwell et al., 1990; Zlatev et al., 1992) and aerosol dynamics including chemistry (Ackermann et al., 1998; Meng et al., 1998; Wexler et al., 1994). Some aerosol models employ aerosol size distribution as a simple function (lognormal, gamma distribution, monodisperse spectrum, etc.). Another approach is used in the aerosol models where the aerosol size distribution is described by non-equilibrium distribution functions (Aloyan et al., 1997; Aloyan, 2000; Meng et al., 1998). In Binkowski and Shankar (1995), a regional aerosol model is described including primary emission, three-dimensional transport and chemistry of sulfuric aerosol particles, based on the oxidation of sulfur dioxide.

In this paper, we describe the structure of the numerical models designed for regional-scale transport and transformation of gaseous pollutants and aerosols in the atmosphere (Aloyan, 1998; 2000; Aloyan et al., 1995; 1997; 2004) as well as present some results of the numerical calculations performed on the basis of these models.

2. HYDRODYNAMIC MODEL

The mesoscale nonhydrostatic hydrodynamic model is based on the equations of atmospheric thermo-hydrodynamics, written in a divergent form in the Cartesian coordinate system and with a terrain-following transformation (Aloyan et al., 1995; Penenko and Aloyan, 1985). The horizontal turbulent exchange coefficients for momentum, heat, and moisture are determined using the Reynolds stress tensor, and the vertical turbulent exchange coefficients are obtained from a (k-ε)-model. The structure of the lower atmospheric layer is described by the Monin–Obukhov similarity theory and the Businger empirical functions. The earth-surface temperature is calculated from the balance equation and the equation of heat and moisture distribution in soil.

3. TRANSPORT MODEL

The basic equations for the concentration change rates of multicomponent gas species and aerosols are represented as (Aloyan, 2000):