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EFFECTIVITY OF ABATEMENT STRATEGIES: PHOXA

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ABSTRACT

The concept and set-up of PHOXA - Photochemical Oxidants and Acid Deposition Model Application within the Framework of Control Strategy Development - is described in detail. The three branches acid deposition, photochemistry and data base and their mutual connections are presented. Main emphasis is given to the data base including the emission data base part of the project, being essential to make further applications in the other branches possible.

To demonstrate which result can be expected from the project in the near future, some calculations are presented for a photochemical episode.

INTRODUCTION

The German and Dutch governments have a long history in joint studies and research on air pollution.

In the beginning of 1983, the two governments decided to start a combined project to evaluate and quantify large scale air pollution phenomena, especially acid deposition and photochemistry, on a European scale. This project called PHOXA, Photochemical Oxidants and Acid Deposition Model Application within the Framework of Control Strategy Development, has been started January 1, 1984.

The aim of PHOXA is to clarify and quantify the behaviour of acid deposition and photochemistry in Europe, because it is obvious from a number of studies that acid deposition and photochemistry are long range processes covering large parts of Europe.

Because international abatement measures have to be taken to control acid deposition and photochemistry, international projects should be set-up to study acid deposition and photochemistry. In these projects as many countries as possible should co-operate and experts from different countries should work together. Among these experts consensus should be reached about the best available knowledge and how to apply this knowledge to arrive at a system by which the effectivity of proposed abatement strategies can be evaluated.

By the end of 1984, the Commission of the European Communities formally joined the PHOXA project, the OECD followed in the course of 1985, and in 1985 also Scandinavian and British institutes. Close relations exist with the EMEP project.

THE PHOXA PROGRAM

The PHOXA program is subdivided into four strongly related branches with the responsibilities indicated below:

- Photochemical Oxidants: The Netherlands/TNO
- Acid Deposition/Application of simpler models: Federal Republic of Germany/TH Darmstadt
- Acid Deposition/Application of complex models: Federal Republic of Germany/FU Berlin
- Data Bases: Federal Republic of Germany/Dornier System; The Netherlands/TNO.

The following items are of main interest:

(a) Modeling area

According to the long-range transport phenomena involved, a modeling area covering almost entirely North-Western Europe has been chosen. The borderlines of this area are: 10° longitude West, 24° longitude East, 47° 30' latitude North, 60° latitude North. The area Covers 3.129.000 km^2.

As can be seen from Fig. 1, most of the main emission areas of Western Europe are contained within the model area, which prevents the atmospheric processes occurring inside from being dominated by the fluxes across the boundaries of the model area.

For modeling purposes the area is covered by a latitude/longitude grid with a grid resolution of 1/2° longitude x 1/4° latitude which gives 3400 grid elements each with an area of approximately 30 x 30 km^2.

Fig. 1 shows also the relative location of the PHOXA area to that covered by the ECE/EMEP project.

Within a cooperation with OECD the PHOXA area will be extended to the North as shown by the dashed line in the Figure 1.

(b) Dispersion models

In PHOXA several dispersion models are applied from rather simple models to more sophisticated ones up to highly complex models. Depending on the specific question, the most suitable model will be used.

Concerning photochemical oxidants the investigation of high concentration episodes is of major interest at present whereas for acid deposition episodic as well as long-term calculations are performed.

The following models are applied:

A) Photochemical Oxidants (Episode Calculations)

Regional Transport Model III (RMT III Model) developped by Systems Applications Inc. USA. This model contains a rather detailed chemistry module, based upon the carbon-bond concept.

B) Acid Deposition

B1) SO_2 and reaction products

- Episode calculations
  - TDMB grid model (TH Darmstadt)
  - RIVM grid model (Rijksinstituut voor Volksgezondheid en Milieuhygiene, Bilthoven)
  - Transport and Deposition of Acidifying Pollutants (TADAP) model, Environmental Research and Technology, USA. The development of this highly complex grid model has been sponsored by Ontario Ministry of Environment, Environment Canada and Umweltbundesamt, Federal Republic of Germany.

- Long-term calculations
  - TDMB grid model (TH Darmstadt)
  - EMEP model (MSC-West, Oslo).

B2) NO_x and reaction products

The process of selecting the appropriate models for episodic and for long-term calculations is still under way.

c) Periods selected for calculations

Within the present phase of PHOXA the models will be applied to the following time periods which have been selected according to concentration/deposition measurements out of the period 1980 - 1983:

- Photochemical oxidants
  22.07. - 26.07.1980 (PHOXA)
  29.05. - 02.06.1982 (PHOXA/CEC)
  03.06. - 06.06.1982 (PHOXA/OECD)

- Acid deposition
  Episodes:
  26.02. - 01.03.1982 (simpler models)
  20.02. - 11.03.1982 (TADAP)
  Long-term: 1982.

It should be stressed that for model validation purposes the investigation of a large variety of different time periods, showing different characteristics, is required.

d) Data bases

For model applications data bases have been established concerning emission, meteorology, ambient air concentrations/deposition and land use.

The emission data base comprises the following substances: SO_2, SO_4^{--}, NO, NO_2, CO, NH_3^+, anthropogenic VOC emissions (split-up in different categories) and VOC emissions from forests. The data base shows a degree of differentiation in terms of source types which allows to assess in detail the contribution of different source types to concentration and deposition levels.

The base year of this data base is 1980. Special programs make it possible to create data bases for other years and for specific episodes by including temperature influences and operating procedures for major sources.

At present a detailed comparison is carried out between this PHOXA emission data base and the inventories obtained by the OECD and emission information obtained by the Commission of the European Communities.

The meteorological input required depends on the models applied. In principle, there are two ways to create the meteorological input:

- by deriving it from observations
- by using a meteorological prediction model.

Both methods are applied within PHOXA.

For the SAI-RTM III model the wind and mixing height fields have been created by the Royal Dutch Meteorological Institute, the fields of the other parameters by Free University Berlin. The meteorological input required by the ERT-TADAP model for acid deposition calculations is entirely derived from the weather prediction model of the German Weather Service, called EUROPE-Modell.

In order to derive initial and boundary conditions and for model validation purposes measured concentration and deposition data are quired.

Within this data base the following quantities for a number of suitable measuring stations are assembled:

- concentration of gases:
  SO_2, NO, NO_2, O_3, PAN
- concentration of aerosols:
  SO_4^{--}, NO_3^-, NH_4^+
- precipitation:
  SO_4^{--}, NO_3^-, NH_4^+, Cl^-, H^+, pH.

The data have been submitted by state agencies and by the Chemical Co-ordinating Centre of EMEP in Oslo.

Concerning model validation there is no doubt that a model which aims at supporting control strategy development has to be validated. Also the uncertainties involved in model applications have to be known quantitatively. The present procedure of comparing calculated volume - averaged quantities with the corresponding quantities derived from point measurements can only be considered as a first step towards a more comprehensive and systematic validation approach. Especially the validation of long-range transport models showing a high degree of complexity requires the solution of a variety of methodological problems. Consequently, PHOXA has started the development of a validation framework for its dispersion models.

Land use information is required

- to derive micro-meteorological parameters
- to derive dry deposition velocities and
- to calculate biogenic emissions.

The land use data base for PHOXA contains the following categories:

01 water surface
02 cropland, arable land
03 meadows, grassland
04 permanent crops
05 built-up areas
06 deciduous forest
07 conifers
08 mixed forest
09 bare soil
10 wetland.

Per grid cell the percent coverage of each of the above categories is given. From their distribution a mean roughness length and a mean dry deposition velocity are calculated per grid cell.

FIRST, PRELIMINARY, RESULTS

After having established the input data bases - which was quite a time consuming work of roughly 2 years - first results have been obtained by carrying out calculations for a five-day photochemical episode in 1980, 22-26 July.

Fig. 2 and Fig. 3 give two examples for the results obtained. Fig. 2 shows a comparison between calculated and measured ozone concentrations within the entire study area for a specific hour. It can be seen that the structure of the measured and the calculated concentration field is quite similar and that the calculated maximum corresponds - in terms of height and location - with the measurements.

Fig. 3 shows the time series on an hour-by-hour basis of the calculated and the measured concentrations for the monitoring station Langenbrügge in the Federal Republic of Germany. Again, the model shows quite good predictive skills.

In addition to the demonstration of the model's skill to reasonably simulate the distribution of ozone in space and time, the following main conclusions from the results obtained uptil now can be drawn:

- During extended time periods rather high ozone concentrations may occur within the study area. These concentrations may exceed 100 ppb.

- The area affected by the high concentrations may cover large parts of the study area. This is a clear-cut indication that the ozone problem is a multi-national problem in Europe with corresponding policy implications.

The results are at present subjected to a thorough investigation which includes sensitivity analysis. More definite results will be obtained in the near future. This applies also for the acid deposition branch of PHOXA.

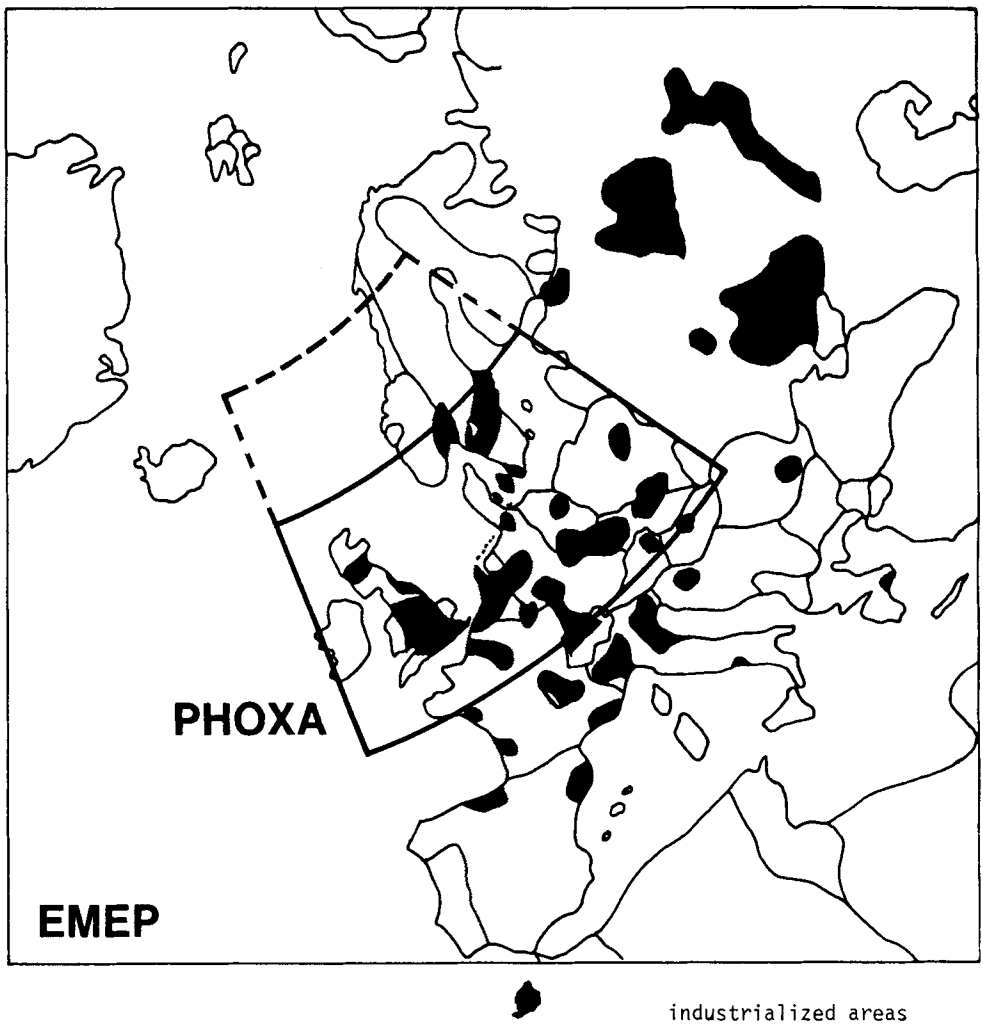

Fig. 1: PHOXA and EMEP study area

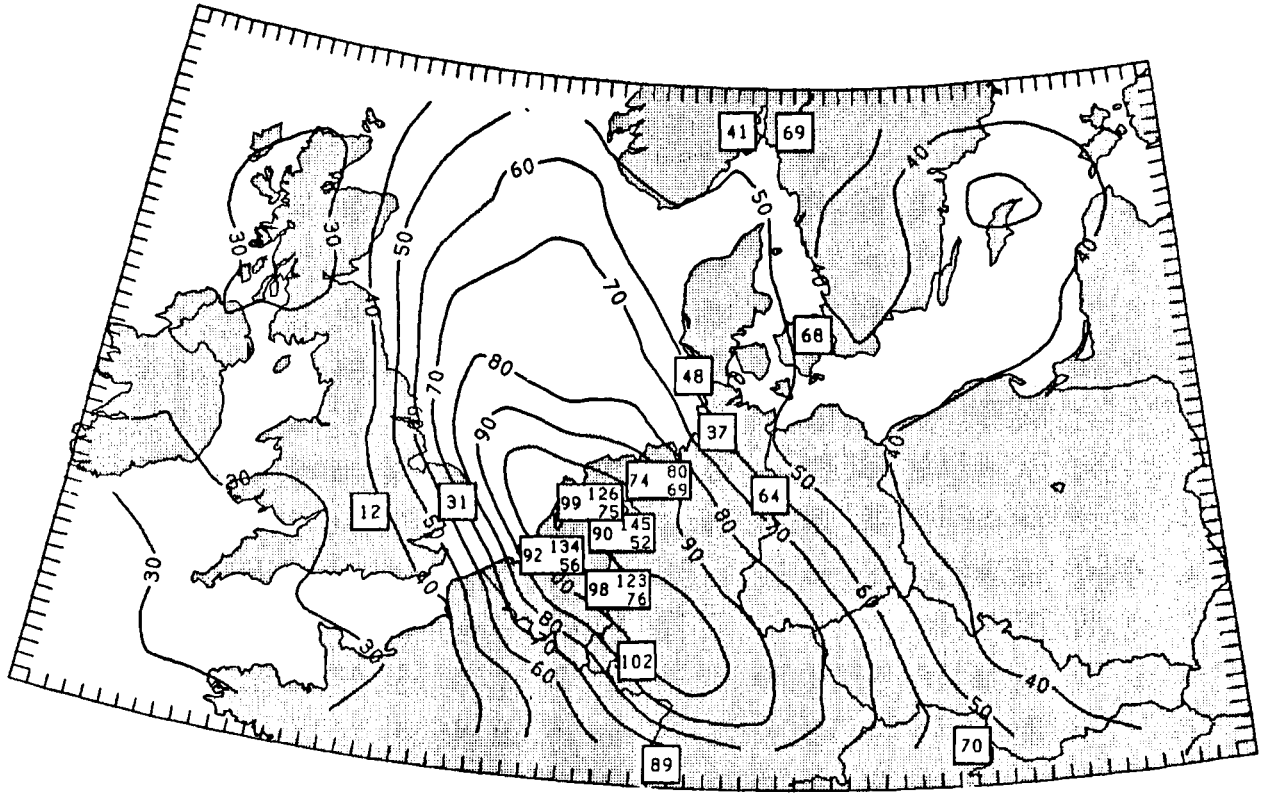

Fig. 2: Hourly Averaged Predicted Mixed-Layer O3 Concentrations (ppb)
With Inserted Observations
For Hour Ending 1800 on 7 / 26 / 80

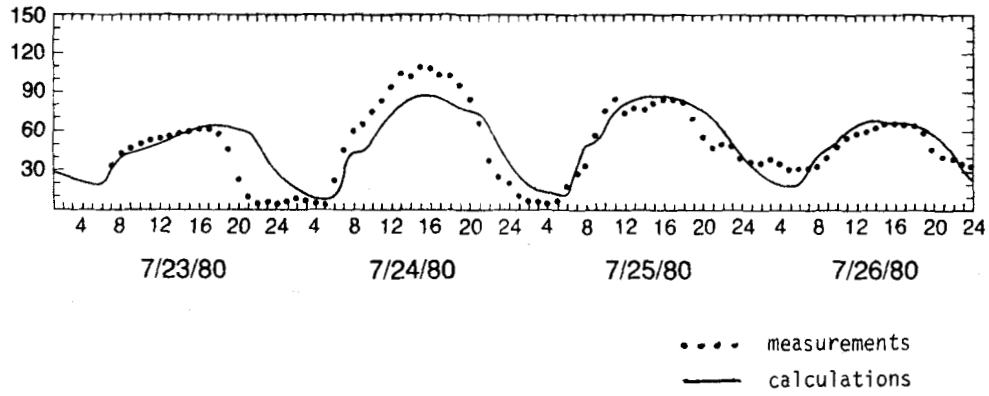

Fig. 3: Calculated versus measured concentrations of ozone (hourly values) for Langenbrügge, Federal Republic of Germany