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# MODELS AS TOOLS FOR ABATEMENT STRATEGIES - AIR QUALITY MANAGEMENT APPROACH

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## ABSTRACT

This paper describes the uses of dispersion and reaction models with particular reference to their role in the regulatory decision making process of air quality control. The features of an AQMS are described. This is followed by a discussion on the need for a critical evaluation of the performance of models especially when used in appraising air quality control strategies.

## INTRODUCTION

This paper is intended to set the scene for this session on the role of modelling as a tool for the development of abatement strategies and to serve as an introduction, providing a back-drop to those papers which will follow and discuss individual aspects of modelling in more depth. This paper therefore will discuss in broad terms the role of air pollution modelling in the overall air quality management system. In the first instance a brief discussion of the various reasons for undertaking air pollution modelling will be given, and we shall see that modelling as a direct component in the pollution control decision making process is only one of several uses of air quality models. This discussion will be followed by an outline of the concept of an air quality management system, involving some brief examples of different implementations of such a concept in various countries. In using air pollution models it is obviously important for the users of both the models and users of the results (who are not necessarily the same) to have an appreciation both of the scope of applicability of the model(s) in question - that is to know whether or not a model is being used in a situation for which it was designed - and of the confidence which the decision makers can place in the results of the models. Both these topics will be discussed below, somewhat selectively as both subjects, especially the latter issue of the errors, uncertainties and sensitivities inherent in models could be (and have been) the subject of conferences in themselves. Examples of the use of models in various situations will be given using examples of urban and longer distance scales and involving primary and secondary pollutants.

On a point of terminology, in this paper the term "air quality" will be used in a broad sense to include both air concentrations and depositions, both wet and dry, of gaseous or particulate pollutants.

## THE USES OF AIR POLLUTION MODELLING

Air pollution models are constructed to simulate the action of the physical and chemical processes occurring in the atmosphere on a source or sources of pollutant emissions. This can be carried out with varying degrees of complexity over a range of time and distance scales, but the chief reasons for performing modelling calculations are one or other (or combinations of) the following:

- Research - to evaluate our quantitative understanding of the important physical and chemical aspects of the problem. These investigations generally result in further questions and in the need for model development and here two approaches are possible. One may wish to develop a model which while simulating the major physical and chemical features of the system, is relatively simple. The reasons for this approach may be philosophical, accepting that a full description of the chemistry (in both gaseous and aqueous phases in the acidification problem for example) and the physics (of cloud formation, rain and wash-out in the same example) will not be feasible; or equally important that the input data required to specify emissions and the atmospheric parameters on sufficiently well-resolved time and spatial scales may not be available. The reasons may also be practical in that sufficient computer power for a more complex model may simply not be available. On the other hand, a more detailed approach may be taken whereby one attempts to include explicitly as much of the detailed physics and chemistry of the system as is practicable given the available computer power. There is neither time nor space here to debate these two approaches but suffice it to say in the context of a research tool, the demands on a model may be different from those required in an operational model used in an AQMS or similar.
- As a supplement to monitoring and in network design - air quality monitoring is an expensive task both in terms of capital and manpower and modelling can often be profitably used to estimate concentrations or depositions in areas where for economic or other reasons monitoring is impractical. This interface of monitoring and modelling places significant demands on model validation - a topic which will be discussed below. Similarly the use of dispersion models as an aid in the rational design of monitoring networks can be a very powerful method for ensuring that the maximum benefit is obtained from the outlay of the networks. This approach has been used successfully by WSL in the design of the UK Rural Network for $SO_2$ and also, in conjunction with other information, in the design of the UK network for monitoring compliance with the EC $NO_2$ Directive.
- In assessing the impact on air quality of future emission scenarios - this can take two forms, one as a single source or single development assessment for example in a form of Environmental Impact Assessment, or the other in a wider

national or international context where for example future forecasts of national emissions and their impact on national and transboundary air quality may be required. The papers following in this session will discuss this application which is (together with the next point) often of most interest to those concerned with the decision making process. It is also, as will be discussed later, an application which places considerable demands on the models and also on their developers and users, particularly as one moves away from the relatively simple linear air quality models of the Gaussian type applied over ~10 km distance scales to urban air quality problems, to the more detailed, often non-linear problems involving longer time and distance scales, complex chemistry, wet and dry deposition.

• Identification of cost-effective control strategies - this is often very closely linked with the previous point but is worth highlighting on its own because of the importance of the issue. In the previous paragraph, one may wish to investigate future scenarios over which one can exercise little control. However when a choice of options is open then it behoves the decision maker to employ a rational evaluation of these options. Numerical deterministic models offer a rational method of assessing future air quality, and coupled with adequate information on control and abatement technology costs can provide a powerful tool in assessing control strategies. However care must be taken in using models in these roles so that they are not simply used as a "black box" which provides unquestioned results for a series of input scenarios.

Air pollution models then can provide very valuable information to the decision maker when used in a rational manner and are probably at their most effective when used in an integrated way with scientific analyses of the rest of the air quality mangement process, and this will be discussed briefly in the next section.

## AIR QUALITY MANAGEMENT SYSTEMS

The management of the factors determining air quality is a complex process and the various methods used by different countries reflect the priorities and problems of each nation. In recent years, particularly with the increasing use of air quality standards in Europe and elsewhere, attention has turned to the formal concept of an Air Quality Management System in which all the factors determining air quality are considered in an integrated way. The definition and description of an AQMS has been the subject of a NATO/CCMS study (ref. 1) so only a brief description will be given here. A schematic outline of the components of the system are shown in Figure 1. It should be emphasised that this is a formal definition - in practice considerable differences in implementation of such a system will occur with varying degrees of formality.

However, regardless of the way in which assessment and control mechanisms are written into national air quality management practices, sound scientific and technical information on each stage is essential before rational decisions can be taken.

Controls and standards can be applied at various stages of the system - for example fuel/product standards can be applied as in the case of the lead content of petrol and the sulphur content of gas oil, both of which are the subject of EEC Directives. At the plant stage control/abatement technology can be applied and it is in the link between this stage and the air quality/deposition stage at the heart of the system that the role of dispersion modelling is paramount.

It may be helpful to illustrate some implementations of AQMS in different countries as examples of the different approaches which may be adopted. The intention here is not to give an exhaustive or definitive account of such systems and approaches but simply to illustrate some salient features in the present context. Some national systems were described in more detail in an earlier NATO/CCMS report (ref. 2).

In the USA for example, the system is founded on the air quality standards (AQS) for the regulated pollutants, so that while emission limits can be set on plants these are determined such that the AQS are not breached. The means of achieving this assessment is a model, so that here models are very much an integral part of the process and indeed evaluation and accreditation of models for appropriate roles is seen as an important task within the AQMS.

The system adopted by the Federal Republic of Germany contains provision for emission standards (for a large number of substances), and for air quality standards on both long and short (yearly and half hourly) timescales. Furthermore there is the requirement that emissions should be kept as low as possible by the application of best available technology to emission, product and equipment standards. It is also a requirement that the contribution to ambient air concentrations from a single stack should not be higher than about 1-2% of the air quality standards. This requirement necessarily involves the use of models.

The approach of the Netherlands offers another example, in that as well as air quality standards, national emission ceilings for $SO_2$ (0.5 MT $a^{-1}$), NOx and $NH_3$ have been set, which in turn lead to the setting of emission standards for appropriate plants. Furthermore targets for the maximum deposition of acidic species have been set amounting to 1400 effective acid equivalents per hectare per year from $SO_2$, 900 from NOx and 690 from $NH_3$.

The foregoing discussion has been concerned with national AQMS and their implementation. In recent years the problem of transboundary transport of air pollution and the acidification issue, with which this meeting is concerned, has become increasingly important. There is no difference in principle between the management of air quality (in the wide sense) at the supra-national level as outlined in Figure 1 and at the domestic level although clearly in practice this may not always be a straightforward process. Nonetheless the requirement for sound scientific and technical information on each of the stages from fuels and raw materials, through plant technologies to the resulting air quality and effects is still paramount. The role of models in this international process is still central and fundamental in answering the important questions, firstly if one wishes to reduce or ameliorate the "effects" be they aquatic acidification, vegetation damage etc, what is the required reduction in air quality/deposition necessary to achieve this? and secondly what is the most cost-effective emission reduction of precursor pollutants which will achieve this reduction?

In the past most attention has been primarily focussed on the second question, models being used to predict air quality from a series of emission control or fuel use change scenarios. This for example is the objective of the PHOXA/CEC/OECD exercise to be described in more detail in a later paper to this meeting. In the acid deposition context one of the most important questions currently being investigated is the form of the relationship between emissions and depositions of acidic species, in particular the extent to which non-linearities in the gaseous and aqueous phase processes affect the proportionality of this relationship. Equally importantly, arguably more so, is the question of modelling the link between changes in air quality and consequent changes in effects. This is a difficult task as many of the mechanisms of aquatic and soil and other substrate acidification are poorly understood. Nonetheless it is essential to have a sound understanding of the likely benefits to the affected targets before embarking on what could be costly control measures. Advances in this area will be viewed with interest and another subsequent paper will address this issue.

So far we have discussed the roles which models can play in an AQMS and in developing rational approaches to abatement strategies. What we shall next consider is a rational approach to the uses of models themselves.

## EVALUATION AND ASSESSMENT OF MODELS IN DEVELOPING CONTROL STRATEGIES

In this section we will discuss the criteria by which the performance of a model in operational use would be judged. All models are approximations, some more so than others, so that validation and sensitivity analyses are essential to ensure sound performance; more fundamentally, the model should be formulated properly in the first place. These aspects will be discussed in the following sections, with particular reference to the acidification/transboundary transport issue.

Model Formulation and Data Requirements

It is a truism, but nonetheless something which can be overlooked, to state that the quality of the results of a model are determined to a large extent by the quality of the input data, which comprise emissions, meteorological/ physical parameters and chemical mechanism/rate constant data. Similarly the construction of the model in its physical and chemical mechanisms should be such that the major features of the problem in hand are treated on the appropriate time and distance scales. For example the detailed description of small scale turbulence in a building wake, of prime importance in a street-canyon model, can be more simply treated in an urban scale (1-10 km) model or longer range model, using a semi-empirical dilution term.

Emissions data should be available on the temporal and spatial scales appropriate to the problem. The calculation of annual average air quality requires annual emissions which, although themselves subject to uncertainties which can be large, are generally readily available for the major pollutants $SO_2$ and NOx although $NO_2$/NOx ratios are not always well defined. Photochemical models require emission data on individual hydrocarbon species and even in annual terms these are often only very approximately known and until the recent OECD MAP exercise, no comprehensive emission data on individual hydrocarbons have been available in Europe. For shorter time scales, of the order of days as required by the Norwegian/EMEP sulphur deposition model, or hours which the PHOXA/SAI model requires, some method of estimating from annual values is often required. Daily space-heating emissions for example can be fairly confidently estimated using the degree-day approach and this is employed by the Norwegian/ EMEP model, while in other areas vehicle emissions can be related to traffic statistics which are often available at an hourly level in major urban areas. It is important to quantify these short timescale variations as factors of 2-3 from the long-term average can be achieved. Moreover it is important to specify correctly the phasing of short term variations in emissions and meteorology - for example short period traffic emissions can peak in the early morning (~8-9 am) when wind speeds and mixing heights are low, leading to concentrations many times a daily or annual average.

The spatial resolution of the model is also a major constraint. Both Eulerian and Lagrangian transboundary models require the specification of a grid-cell size which imposes demands on the specification of emissions and also means that certain sub-grid scale physical and chemical processes must be treated approximately. Typical grid sizes for urban air quality models are ~1 km while the EMEP sulphur deposition model uses a grid size of ~150 km. The photochemical SAI model has been used in the USA with a grid size of ~18 km and in the PHOXA and CEC/OECD applications the grid sizes are ~25-50 km. It is not always easy to obtain spatially resolved emission inventories for all the pollutants of interest. Such data are now generally available for $SO_2$ and NOx, and WSL has developed UK inventories at ~20 km resolution for these pollutants. However as noted above in the national context, spatially disaggregated inventories of individual hydrocarbons are more difficult to obtain. Recently a European inventory of $NH_3$ emissions for 1982 has been developed (ref. 3) on a 75 km basis and a similar inventory for the UK on a 10 km grid has been produced by ApSimon and Krause (ref. 4).

The requirement to use large (>10 km) grid sizes in long range transport models has other important implications in that sub grid square processes must necessarily be treated or parametrized in an approximate way. For example in many applications, large point source emissions are assumed to be instantly mixed over the volume of the grid cell. While this may not be a serious approximation at large downwind distances for an inert pollutant, near field concentrations will probably be poorly predicted. Likewise the concentration gradients which exist in reality will not be modelled directly with what may be important consequences for chemically reactive species. In the acid deposition context subgrid scale effects of enhanced wet deposition can also be important. Moreover when the validation of the model is being considered it should be remembered that in most cases measurements are made at a point or in the case of an aircraft a line, and calculated values are grid-cell averages over a volume so that comparisons are thus not direct; this is also discussed in the next section.

## Validation and Sensitivity of Models

In an ideal situation of unlimited resources, a thorough validation of a model would be large exercise involving validation of the input data on emissions etc as well as a thorough comparison of modelled and measured values over a wide range of locations and a long enough time period to cover the major variations in concentrations which might be expected to occur. In practice very detailed exercises are often not practicable particularly on an international scale. However good coverages (in time and space) of measured data exist so that considerable steps can be taken towards full validation of models. Methods of model evaluation (and the term is used here synonymously with validation although the two can be very different) have been studied in some detail by the American Meteorological Society and EPA (refs 5,6) although a considerable amount of complexity can be generated by calculating a large number of statistics, often at the expense of understanding a model's behaviour. It is often enough to plot the calculated and observed quantities simply as (x,y) points, as a time series and if appropriate, as frequency distributions and pollution roses. Model performance can often be usefully expressed as a single parameter

$$M = \Sigma\ (C_{oi} - C_{ci})^2/\Sigma\ (C_{oi} - \bar{C}_o)^2$$

which is minimised for optimum agreement between calculated ($C_c$) and observed ($C_o$) concentrations.

Typical plots of $C_{ci}$ vs $C_{oi}$ are shown in Figs 2 and 3 for the Norwegian/EMEP model calculations of $SO_2$ in air for 1978-82 (ref. 7) and for calculations of wet deposition of sulphate (ref. 8). From the scatter of the plots an indication of the level of agreement is obtainable.

The problem of point measurements compared with volume averaged model results has already been noted and it is important therefore to have some idea of the spatial representativity of a point measurement. This has been addressed by Barrie (ref. 9) who attempted to quantify the uncertainty (point measurement error plus area representativeness) in annual $H^+$, $SO_4^{2-}$ and $NO_3^-$ concentrations as a function of network spacing in the Eastern USA and these are shown in Fig. 4.

Predictions of models can also be expressed in a statistical or probabilistic sense as shown in Fig. 5 where a summary is given of urban $SO_2$ concentration results from WSL's model applied to urban areas in the UK. Recently Derwent (ref. 10) has outlined a method whereby given the frequency distributions of likely values of model input parameters, the frequency distribution of the model results can be calculated, so that results can be presented in a probabilistic manner.

Whatever methods are chosen to quantify a model evaluation, simplistic routine calculations of a series of statistics are not by themselves sufficient, and can be misleading. An investigation of the behaviour of the sub-models is essential. For example does the meteorological sub-model predict or use parameters (boundary layer height, wind fields, cloud cover or radiation fluxes, wind speeds etc) which are realistic? Modelling conservative or slowly reacting species can assist in this evaluation, and certainly the sensitivity of the model output to realistic uncertainties in the input values of these parameters should be investigated. In the use of photochemical models to evaluate control strategies for oxidant concentrations, the performance of the chemical sub-model is of major importance (although the specification of the physical parameters can play an important role in determining oxidant concentrations). Care must be taken in such cases in asking the right questions of models - in the oxidant example it is important to be clear on where, in relation to major precursor emissions, one wishes to minimise oxidant concentrations since a control strategy optimal for the near field will in general be different from the strategy further downwind. Likewise at a given location, control strategies or predictions of changes in ozone concentration following emission changes, will differ from one chemical scheme to another. Full validation of models in these applications is often not possible, but some recent work by Dennis (ref. 11) using three versions of the Carbon Bond Mechanism in the SAI model showed the need for a systematic investigation of the sensitivity of control strategies to different chemical schemes and also the need to model a range of ozone episodes, for while the three schemes on average predicted similar ozone changes from 1976 to 1979 in Denver (7.6% - 10.0%), on some days the spread was larger, (2.4%-16.8%) in the worst case.

It is clear then that in order to assess the performance of models in a regulatory application, it is essential to evaluate the performance of the model in situations similar to that in which it is to be applied. For example while it may be valuable to evaluate predictions of the variation of ozone concentration under different meteorological conditions with a fixed emission inventory, this may not necessarily offer relevant information on the ability of the model to predict the effect of emission changes on ozone concentrations. There is a need for greater emphasis to be placed on model evaluation in a regulatory context if rational decisions are to be taken. This has been highlighted by some recent work of Walker (ref. 12) which suggests that despite stringent emission controls in California and Texas, there may have been no significant changes in ambient ozone concentratons in these areas.

SUMMARY

We have seen that air pollution models can play a central role in an AQMS and can be powerful tools in the development of rational and cost-effective abatement strategies. Indeed models represent the only quantitative prognostic approach for the decision maker. However models must be used in a critical way, ensuring that they are properly formulated for the task in question and moreover that their accuracy and sensitivity are properly investigated over the range and variation in input conditions (be they meteorological or emission controls) appropriate to the regulatory questions. With wide open critical eyes on the part of practitioners <u>and</u> decision-makers ,models can be a very powerful part of an AQMS.

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are those of the author, not necessarily those of the Department of the Environment.

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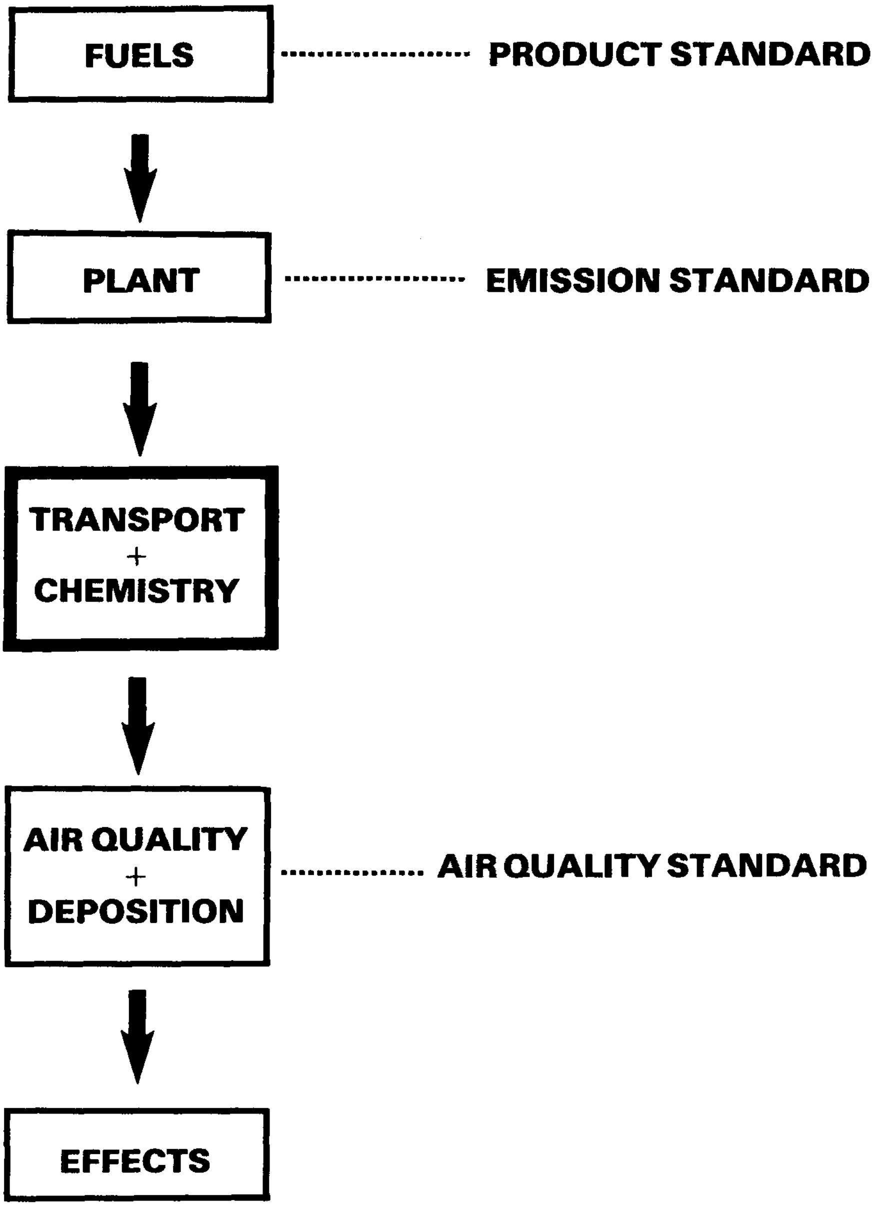
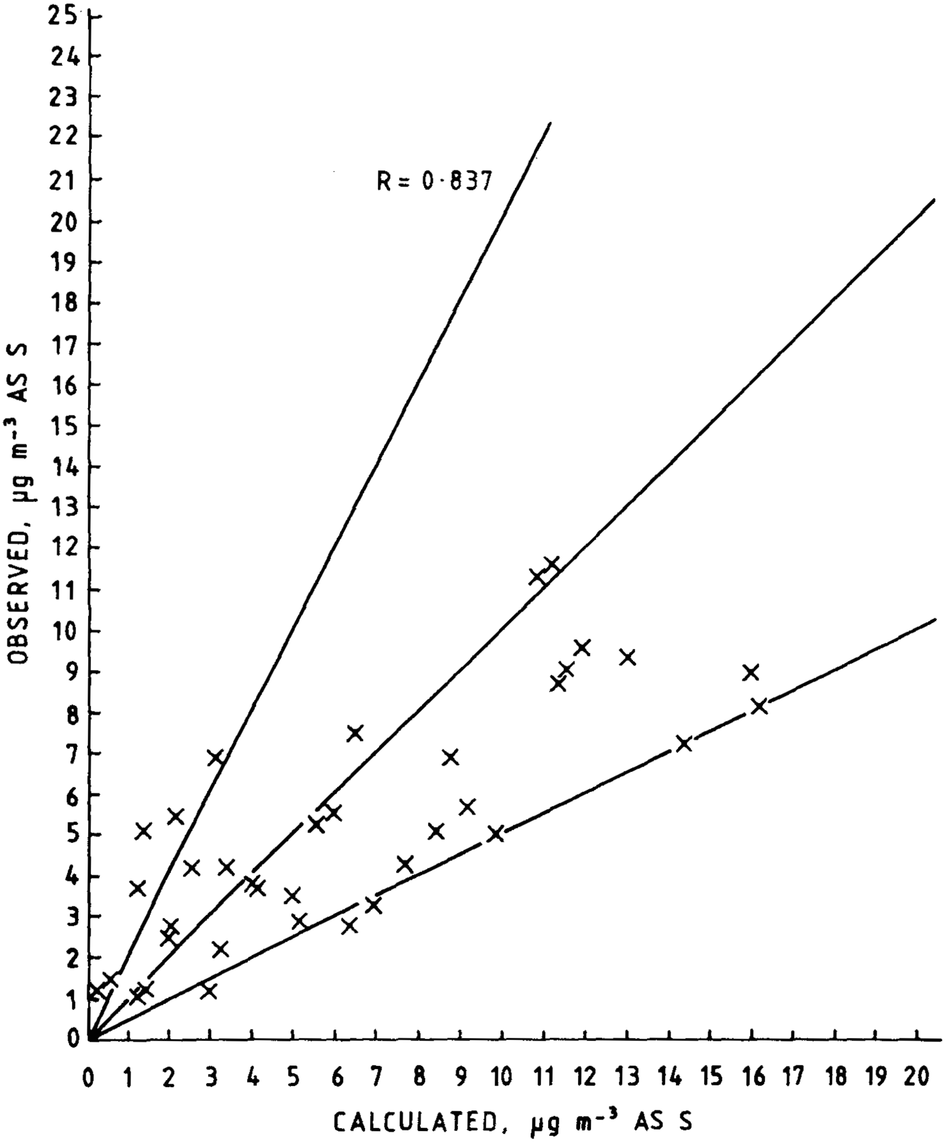

FUELS
PRODUCT STANDARD
PLANT
EMISSION STANDARD
TRANSPORT + CHEMISTRY
AIR QUALITY + DEPOSITION
AIR QUALITY STANDARD
EFFECTS

FIG. 1




EMEP-5 YEARS DATA: 1978 - 1982, $SO_2$ -S AIR CONC.

FIG. 2

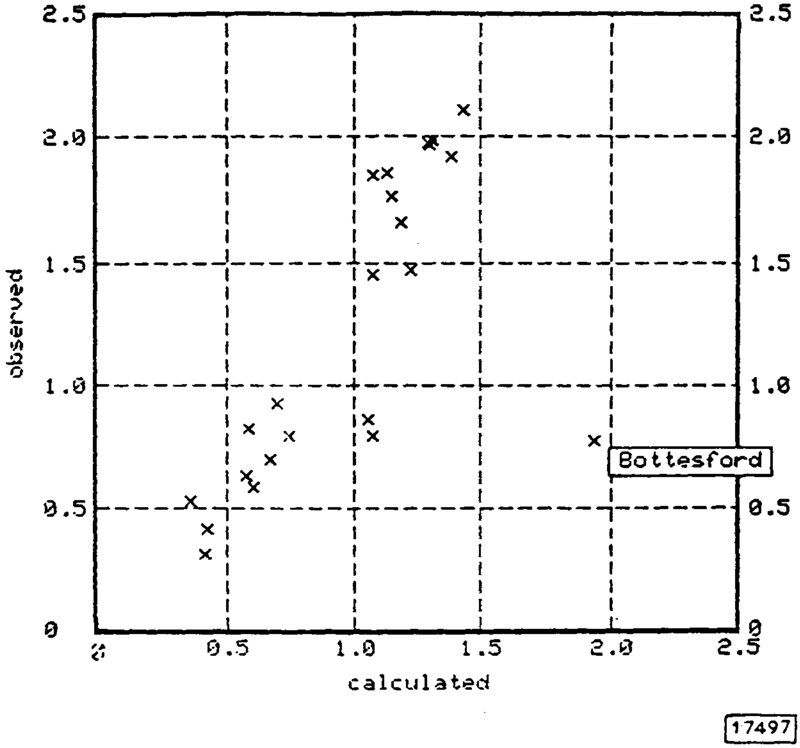
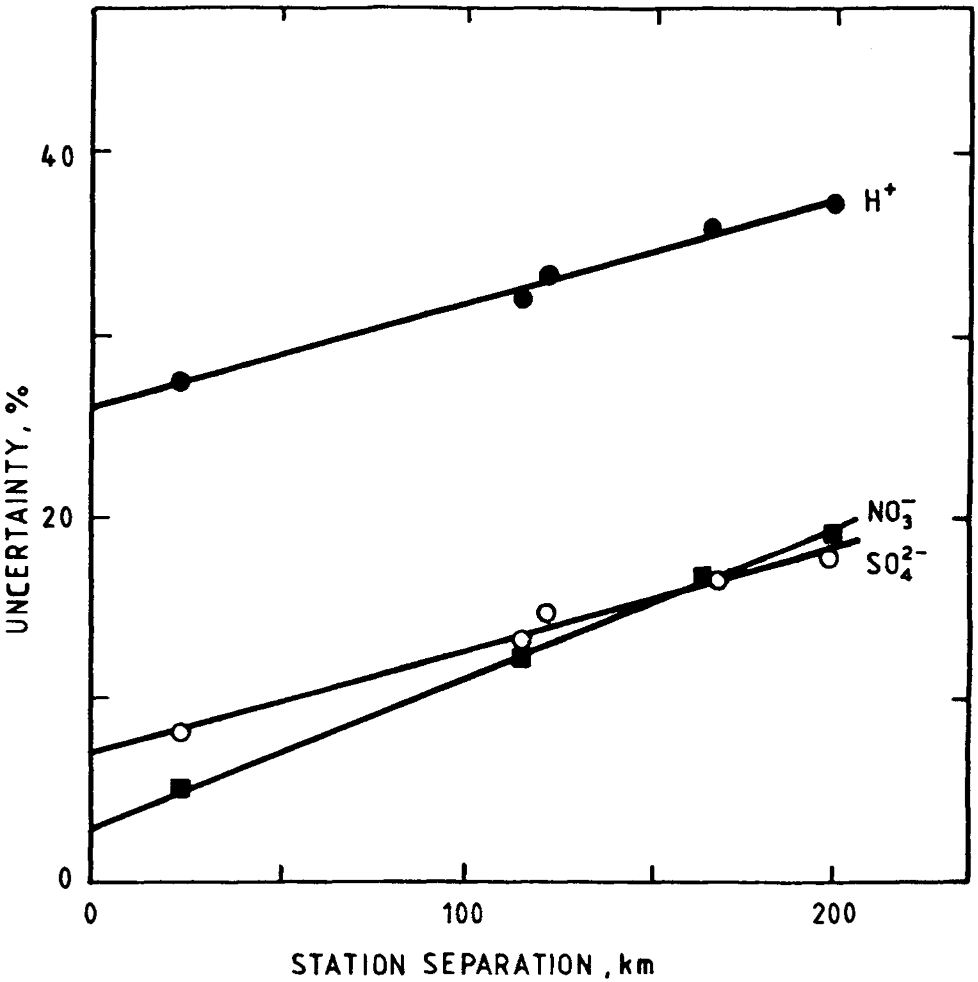
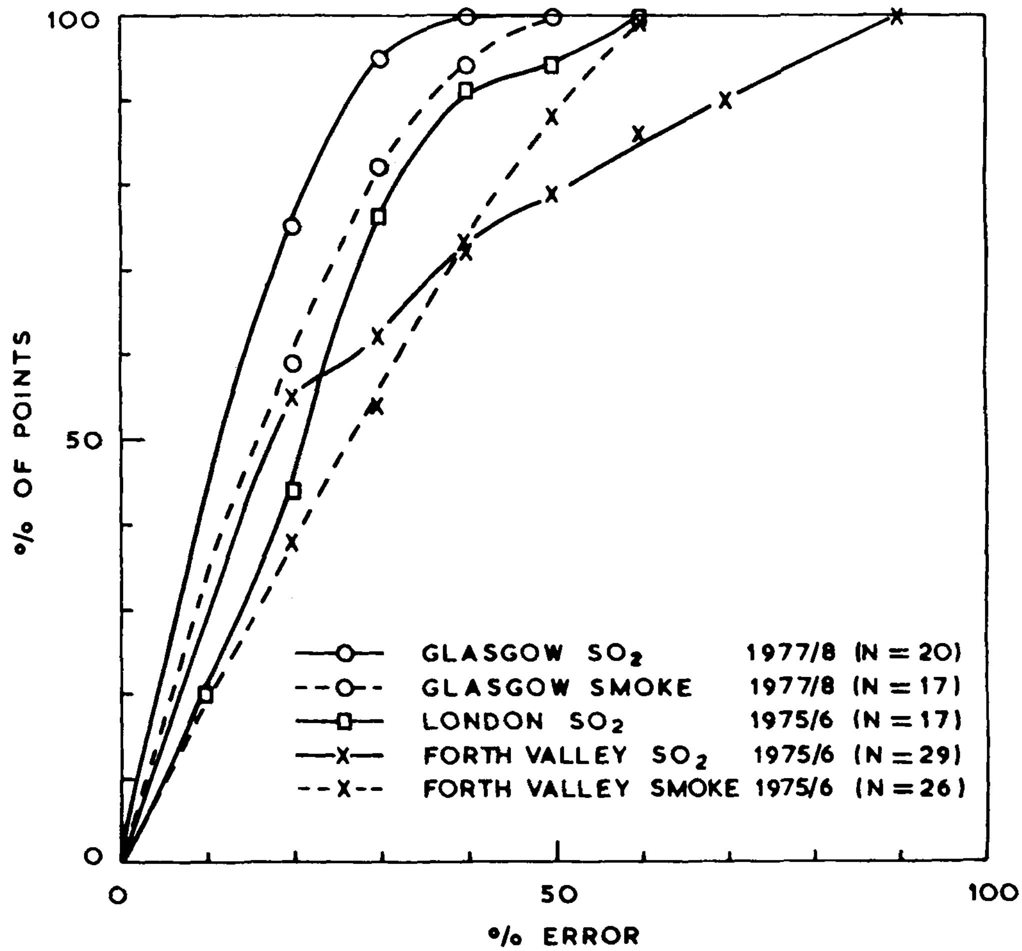



Fig.3 Calculated (including background of 20 $\mu eq\ l^{-1}$) vs Observed Wet Deposited Non-Marine Sulphate, 1983, $gS\ m^{-2}$




THE TOTAL UNCERTAINTY (POINT MEASUREMENT PLUS AREA REPRESENTATIVENESS) IN ANNUAL HYDROGEN ION, SULPHATE AND NITRATE CONCENTRATION MEASUREMENTS IN THE EASTERN UNITED STATES AS A FUNCTION OF NETWORK SPACING (BARRIE, 1983)

FIG.4




PLOTS OF PERCENTAGE OF RECEPTOR POINTS WITHIN PERCENTAGES OF OBSERVED CONCENTRATIONS FOR ANNUAL AVERAGE $SO_2$ CONCENTRATIONS

FIG. 5