AIR QUALITY MODELLING FOR POLICY DEVELOPMENT

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ABSTRACT

Atmospheric models constitute the best tools available for the setting of policy, and may, in some cases, be the only tools that are available. The best examples of their kind bring together all current knowledge of pollutant behaviour in the atmosphere, making it possible to unravel the often complex interactions between pollutants and atmospheric dynamics. They also allow the possibility of evaluating hypothetical changes in emissions and other conditions to evaluate potential abatement strategies, or to assess the impact of proposed new emission sources. This paper provides an overview of mathematical atmospheric models and their application to the development of air quality policy. The paper discusses the types of atmospheric models currently in use, categorized by spatial scale, and the requirements for credible modelling. Issues associated with model validity and accuracy are described and case studies are reviewed to illustrate atmospheric model use in policy development and the need for careful analysis in interpreting model predictions.

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INTRODUCTION

A model may be defined as a representation of reality. The particular representation used in any given case can take a number of forms. Examples include scale models constructed of cardboard or wood to show the appearance of a building or a ship, or the conceptual models of human interaction that we all carry around and invoke many times per day, albeit often unconsciously. However, in the context of this paper the models considered are mathematical representations of the behaviour of pollutants in the atmosphere. The objective of this paper is to provide a description of mathematical atmospheric models, and their application to policy.

Policy is another term which has a number of possible definitions. The particular context required here includes measures designed to control or eliminate atmospheric pollutants to protect human health. In general, "control or eliminate" means "reduce or eliminate the emission of these pollutants to the atmosphere". Other policy issues are, of course, also of current importance, e.g., visibility degradation especially in pristine areas, and impacts on ecosystem health.

The value of models in policy development lies in their ability to provide a quantitative link between pollutant emissions at one or many locations, and the resulting concentrations or doses of pollutants experienced by the human or other receptors, whose health is to be protected. This allows changes in impact resulting from hypothetical changes in emissions to be readily evaluated. Such evaluation is almost impossible to carry out experimentally, either because it is far too costly to shut down a source or sources, and to attempt to measure the concentration changes at the desired receptor locations, or because the assessment is required for a source that is yet to be built. In addition, the complexity of the interrelated chemical and physical processes is such that measurements alone are extremely difficult to interpret without the conceptual framework provided by a model.

To a large extent, the acceptance of models as valuable tools has followed the realisation that an airshed can cover several jurisdictions; emissions from sources in one jurisdiction can and do have impacts on the residents of other jurisdictions. Policy negotiations between jurisdictions are very difficult without a quantitative understanding of the link between the emissions and the impacts. Models used to support such negotiations must be credible. This has driven continued improvements in the science of models, and in their evaluation against measurements.

This paper will summarise the types of atmospheric models currently in use, and the resources required to run them. The very important subject of model accuracy will be discussed and case studies will be presented. In preparing this paper a wide range of current scientific literature has been reviewed. However, this paper is not intended as a comprehensive review of the current state of modelling. Such reviews are available elsewhere, e.g., the two assessment reports produced by NARSTO (2000, 2003) and the paper by Peters et al. (1995).

POLICY APPLICATIONS OF MODELS

A distinction can be made between the use of models in the development of policies, and their use as research platforms. As a research platform a model serves as a framework for current knowledge of the chemical and physical behaviour of the atmosphere. Comparisons of model predictions with measurements then constitute tests of the current knowledge and the way in which it is implemented in the models. In this kind of evaluation model shortcomings can be of greater interest and importance than successes, since they indicate shortcomings in the underlying scientific knowledge and spur advances.

There are at least two major ways in which models can be applied in policy development:

- An appropriate model is applied to the emissions from a source, or group of sources, to predict concentrations at selected receptor locations. These predicted concentrations are then used with a risk assessment/health impact model to predict the health outcomes associated with the emissions.
- A determination is made of what the maximum allowable concentration of a given pollutant should be to be protective of human or ecosystem health. An appropriate atmospheric model is then used to assess what the emissions must be to ensure that concentrations remain at, or below, the desired concentration under all conditions.

Note that application of modelling to one problem pollutant will often provide results which are applicable to others. For example, modelling for fine particulate matter may also generate useful results for ozone, and probably also for visibility.

TYPES OF MODELS

The mathematical models discussed in this paper use data (emissions, meteorology, topography, land use, etc.) in the prediction of pollutant concentrations. Other types of mathematical models exist, particularly receptor models, which use ambient measurements and knowledge of the relative composition of emissions from the relevant sources or source categories to calculate the relative contributions of the sources at the measurement point. Receptor models are valuable in determining such contributions if the required data are available, but can not be used with confidence to predict the effect of reducing emissions from any of the sources, because they inherently assume that there is a linear relationship between emissions and concentrations. They will not be included in the discussion presented here. Further details may be found in NARSTO (2003) and the references cited therein.

Note that the terminology of modelling varies, and may depend on the particular application. The models discussed here may also be described as “chemical-transport models”, “diagnostic” (applied to the current situation) or “prognostic” (applied to a future situation).

The predictive models discussed in this paper may be categorised in many ways. The approach adopted here is to categorise by applicable spatial scale, with further consideration of mathematical formulation, and type of pollutant considered. Examples of current use models will be given in each category.

It is convenient to consider three spatial scales: local, meso- to regional, and global.

Local scale

Local scale modelling is typically used to assess the impact of single sources, or small groups of sources, over distances ranging up to tens of kilometres. Typically the pollutants are emitted from a stack, with an initial velocity, and at a temperature which is generally above that of the ambient air. Under the combined effect of the exit velocity and the buoyancy due to its elevated temperature, the plume rises above the stack top, before being bent over, and transported or advected by the wind. Turbulent eddies in the atmosphere spread the plume out in the horizontal and vertical directions. This dispersion leads to dilution of the pollutant as the plume travels downwind. The process is typically modelled by assuming a Gaussian concentration distribution in the horizontal and vertical directions (Figure 1). The resulting concentration is then given by:

$$C(x,y,z) = \frac{Q}{2\pi V \sigma_z \sigma_y} \exp\left[\frac{-y^2}{\sigma_y^{\,2}}\right] \exp\left[\frac{-z^2}{\sigma_z^{\,2}}\right] \qquad (1)$$

where
- C = concentration at point x, y, z
- x = distance along plume centre line
- y = horizontal distance from plume centre line
- z = vertical distance from plume centre line
- Q = emission rate
- V = wind speed
- σ_y, σ_z = dispersion coefficients in the y and z directions

Note that σ_y and σ_z specify how much the plume spreads, and are derived from theoretical arguments or empirical fits to observed data. They are increasing functions of x, and their numerical values are dependent on the stability of the atmosphere. Because the distance and time scales considered are short, chemical or physical transformation of the pollutants modelled is almost never included in these models.

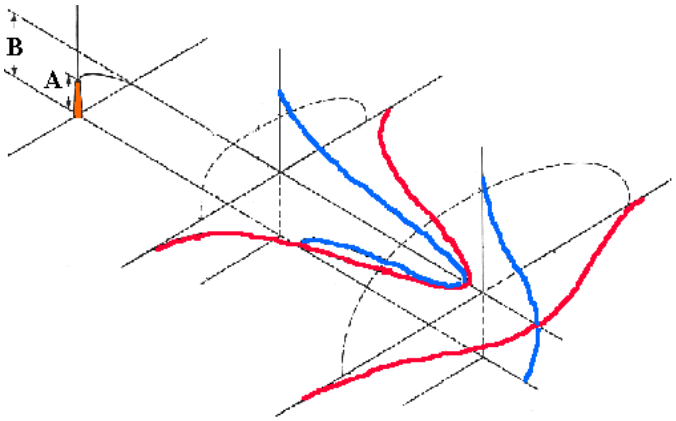

Figure 1: Depiction of Gaussian plume.

Equation 1 represents the simplest case of Gaussian dispersion. Many variations are employed to treat more complex situations, including:

- multiple sources
- impaction of the plume on the ground, or its confinement by topography
- special behaviour under certain stability or boundary layer conditions, e.g., fanning, looping, fumigation, etc.
- the effect of buildings on plume behaviour

Examples of Gaussian type models in current use include ISC and AERMOD in North America, and AUSPLUME used in Australia. The major application for this type of model is in certifying or licensing the emissions from industrial facilities. The appropriate form of the model is run for the facility seeking certification (noting that it may well still be in the design stages), to ensure that the resulting pollutant concentrations are below the relevant air quality standards or criteria, and are thus protective of human and ecosystem health.

A special case of the short term models is in their application in emergency situations, where they are applied in the case of a pollutant leak or discharge of any type. The objective in this case will normally be to define areas in which concentrations are at dangerous levels, necessitating evacuation or other emergency measures. The major difficulty in emergency response modelling usually lies in adequately defining the source emission characteristics. The effective release point may be at ground level, if there is a steady leak from a tank, or if the release material is denser than air. In the case of a fire, on the other hand, buoyancy may lift the pollutants a considerable distance vertically before transport and dispersion begin. It is also usually difficult to determine the rate of pollutant release, and in the case of a fire, even to know what pollutant is involved.

Mesoscale to Regional Scale

Mesoscale to regional scale models consider spatial scales ranging from a few hundred to a few thousand kilometres. These are the spatial scales over which many of the most pressing air pollution concerns are important, and are also the scales which often cross jurisdictional boundaries. Taken together, these facts mean that models on these scales are generally the most important for policy makers. Mesoscale is itself subdivided as meso-gamma (0 to 20 km), meso-beta (0 to 200 km) and meso-alpha (0 to 2000 km). Meso-alpha overlaps with what is usually considered regional scale (up to three or four thousand kilometres). Up to ten or fifteen years ago it was usual to consider mesoscale separately from regional scale, a separation imposed by limitations in the science of modelling and in computer capability. Advances in both make it now possible and convenient to consider both scales together. References to regional scale will be taken to include mesoscale in the remainder of this paper.

There are two major types of regional scale models, depending on the mathematical framework used.

Lagrangian models consider air parcels which travel with the wind (i.e., they are advected). Lagrangian models are

often also referred to as trajectory models, since the air parcel under consideration follows a trajectory defined by the winds, as illustrated in Figure 2. Typical trajectory times for regional scale applications are 3 to 5 days, though longer or shorter times are also used. The trajectories are normally calculated as linear segments, each one covering 3 to 6 hours, with the segment length and direction determined by the average wind speed and direction over the appropriate time step.

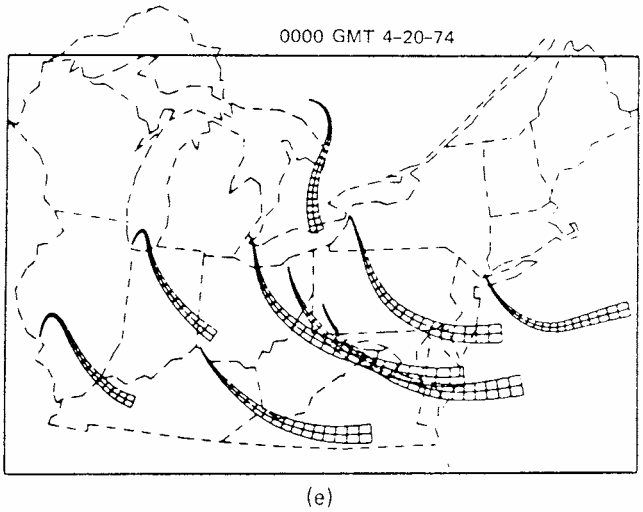

Figure 2: Depiction of a Lagrangian framework for several emission sources in North America.

There are a number of possible variants within the general category of Lagrangian models:

- The trajectory may be run forward from a given source, to evaluate its impact on receptor areas. A new trajectory will be initiated at intervals, e.g., every 3 to 6 hours. Atmospheric variability is such that these trajectories will all be different, so that all affected receptors will be impacted if a long enough time period is followed.
- The trajectory may be run backwards. This actually means that the trajectory is defined in backward steps from a given receptor, and the air parcel is then released from the start point of the trajectory, finishing at the receptor. This approach allows assessment of the effect of all possible emission sources on the given receptor.
- A number of variants deal with the treatment of the air parcel under consideration. For example, it may be considered as a “puff”, which expands during travel, to simulate atmospheric dispersion, or it may be treated as a “wall of cells”, with pollutant mass transferring from inner cells towards outer cells, again simulating atmospheric dispersion. These two methods (and others related to them) allow emissions to enter the air parcel, and chemical and physical transformations to take place within the parcel. A third method treats the emission of “particles”, with a number of releases occurring for each trajectory, but with a random displacement added normal to the trajectory direction. This displacement simulates the effect of dispersion, and the ensemble of particle positions along the trajectory gives the concentration of pollutant at points on or near the trajectory. This last method does not readily allow incorporation of emissions or chemical and physical processes.

Eulerian Models consider a mathematical framework anchored to the surface of the earth, as shown in Figure 3.

Eulerian models are often also referred to as grid models, since the framework is a three dimensional grid, with pollutants being emitted into the grid at the appropriate points. Pollutants travel through the grid, under the influence of the local winds, undergoing chemical and physical transformations as they go. Although a wide range of degrees of complexity is possible in the treatment of individual processes in an Eulerian model, models of the current generation tend to be quite similar overall.

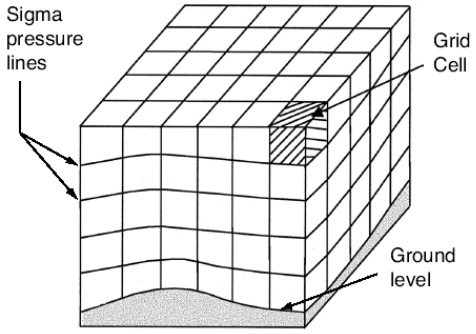

Figure 3: Eulerian modelling framework.

Both types of regional scale models have advantages and disadvantages, as summarised in Table 1.

Table 1. Advantages and disadvantages of Lagrangian and Eulerian models.

	Lagrangian	**Eulerian**
Advantages	• Computationally relatively simple • Especially suitable for small number of sources or receptors • Easy to determine transboundary fluxes	• Able to include treatment of all processes currently considered important. • Non linear phenomena, especially those associated with chemical processes, can be more easily incorporated in a direct fashion
Disadvantages	• Can not readily treat a number of processes, e.g., vertical structure of the atmosphere, including changes in wind speed and direction with altitude, and pollutant transport in layers aloft • If many sources or receptors are considered, computational effort approaches that required for Eulerian case	• Computationally more demanding

Examples of current use Lagrangian models include Calpuff and Hysplit, while Eulerian models would include Models-3/CMAQ, UAM and TAPM.

Global Models

As the name implies, global models consider the transport of pollutants throughout the atmosphere, with no artificial restriction of the domain. Many or most current use global models are Eulerian in formulation; GRANTOUR (Liousse et al., 1996) is a Lagrangian exception. The large spatial extent of these models dictates that the spatial resolution (grid spacing) must be relatively coarse to keep the computational demands within reasonable bounds.

To date, most global modelling has been confined to carbon dioxide and the climate change issue, which also means that chemical transformation is not treated, further streamlining the computation. However, expansion to other pollutants has recently taken place. An example is Environment Canada's global scale mercury modelling (Dastoor and Larocque, 2004).

Processes Treated in Models

Modern atmospheric models, particularly those on the regional scale, treat a number of processes. These are summarised briefly below:

- Emission. Emissions of the pollutants treated by the model must be presented at a resolution (temporal, spatial, chemical, etc.) appropriate to the model. Emissions from both anthropogenic and biogenic sources will be required. Much of the emission information will itself be generated by models, especially for mobile and biogenic sources.
- Transport. Transport involves the movement of pollutants by air motions in the atmosphere. Wind speeds at higher altitudes are generally higher than those at the surface, and the directions are usually different too. Pollutants which have been transferred to higher layers can thus travel considerable distances, in directions which may not be predictable from observations made at the surface of the earth. Vertical movement of pollutants, e.g., by convective processes, can thus be very important. Wind fields may be derived directly from observations, but it is now much more common to obtain them from a meteorological model, which may also provide information on clouds and precipitation, as required for other modelled processes.
- Chemistry. The underlying chemistry of the atmosphere is that of reactive species in the gas phase, driven by sunlight. However, reactions in the aqueous phase (e.g., in cloud droplets) and on the surface of particles must also be considered.
- Physical transformation. The products of some gas phase reactions are condensed solid and liquid phases, taking the form of very small particles. The processes by which these particles are formed, and by which they grow must be included. Particle size is an important parameter, from the point of view of human health impacts, as well as their dynamics in the atmosphere. For example, particles can play a role in the formation of clouds.
- Deposition. Atmospheric pollutants can be deposited to the surface of the earth by dry and wet processes. Dry deposition occurs when the pollutant impacts and is retained on the surface. Wet deposition is the process by which pollutants are incorporated into water droplets or ice crystals and subsequently removed in precipitation.

It may be seen from the above description of processes that modern atmospheric models rely on information provided to them by other models. It is therefore more correct to speak of a system of models, rather than a model, though both terms will be used here.

REQUIREMENTS TO RUN MODELS

A number of requirements must be met before a model or models can be used by an institution or agency. Ironically, acquiring the model itself may be the least difficult of these. This follows from the ready availability of codes for a number of models, e.g., through the World-wide Web. The US EPA in particular has a free distribution policy for many models including Models-3/CMAQ, HYSPLIT, AERMOD, etc.

A number of the important requirements for credible modelling are summarised below.

Choice of model

Even though a model may be freely available, it does not follow that it is necessarily the most appropriate for the situation under investigation. In particular, the science of the model must match the pollutant(s) of concern. For example, if the pollutant of concern is fine particulate matter, the model chemistry must be able to handle reactions of NO_x, SO_2, volatile organic compounds (VOC), ammonia, etc. Reactions in both the gas and aqueous phases must be included, and preferably also heterogeneous reactions taking place on the surfaces of particles. Apart from correct treatment of transport and diffusion, the formation and growth of particles must be included, and the model must be able to track the evolution of particle mass as a function of size. The ability to treat deposition of pollutants to the surface of the earth by both wet and dry processes is also required.

Input data

Modern models require a considerable volume of data. The specific needs reflect the science incorporated in the model, but will typically include the following:

- Emissions. For all sources treated by the model (for each grid square of an Eulerian model) the rate of emission is required for each of the chemical species followed by the model, specifically including each of the VOC species or categories used in the model chemistry, i.e., both anthropogenic and biogenic. These emissions

should relate to the specific time period being studied. A very large effort is devoted to emission inventory construction world wide, but it remains true that there is still considerable room for improved accuracy. In general, emissions of sulphur dioxide are specified with the best accuracy, followed by oxides of nitrogen, then volatile organic compounds. With the need to model fine particulate matter formation and transport, emissions data are also required for primary particle emissions as a function of particle size, as well as emissions of ammonia. Neither of these is particularly well categorised as yet. Specifically, primary particles in small size ranges (e.g., $PM_{2.5}$ or smaller) may be emitted in large amounts from unpaved roads or agricultural operations, but it appears that only a fraction of these emissions are "effective," i.e., are subject to transport. This fraction is not well known. Ammonia emissions are also subject to large uncertainty and it is possible that not all sources are known.

- Geophysical data. Information is required on a range of surface parameters, including topography, land use category and vegetation type. These are generally more readily available than emissions data, and some of them (like topography) do not usually change with time.
- Meteorology. Meteorological information is typically required to drive the transport in the model. This information is needed at several levels in the atmosphere, and must also be for the period to be modelled.
- Initial and boundary conditions. It is usual to specify the initial chemical concentrations for a number of the major species in the model. These will be taken from typical or average values measured, or previously modelled, for the region of interest. The exact values chosen may not be completely critical, as the model will usually be run for some initial, warm up period (typically about two days), so that concentrations in the modelling domain are determined by model processes within the domain. However, poor choice of initial conditions will lead to long warm up times. It is also necessary to specify concentrations at the boundaries of the model, except for global models. It is usual to allow a buffer of two to three grid squares on the edges of the domain for an Eulerian model, within which the concentrations will be determined more by the boundary conditions than by the processes within the model. Again, the exact values chosen for the boundary conditions may not be important, except that poor choices will require large buffer zones, and boundary conditions will be very important for inert substances which are not emitted within the model domain. Note that while it is relatively simple to estimate initial and boundary conditions at the surface based on measurements, these values are also required at higher levels in the atmosphere, where measurements are very much sparser. Current practice, which addresses the specification of initial and boundary conditions is to nest the model. In nesting an initial run is carried out for a large domain at relatively coarse resolution. This is followed by a run at finer resolution for a smaller subdomain, using predictions from the first run to provide initial and boundary conditions.

Computer resources

Modern Eulerian models are very computer intensive. However, modern computers are much more powerful than were their predecessors. The result is that computational limitations, although they still exist, are much less restrictive than they were a decade ago. Many modern models are run on large computer facilities, but others are now run on computer workstations, or clusters of desktop computers, which are within the budget of many institutions.

Practitioners

The need for skilled practitioners to run models should not be underestimated. Many models are now freely available, as noted above. However, the danger exists that these models can produce misleading results, unless their use is overseen by knowledgeable persons. Training of new generations of modellers is therefore seen as a very important component of modelling.

To summarise, many models are now available at little or no cost. However, the establishment of an atmospheric modelling capability carries a non-trivial cost, because of the need to provide appropriate supporting data, computer resources and scientists. Examples of model applications are discussed later in this paper, including two cases illustrating how misinterpretation can occur.

MODEL VALIDITY AND ACCURACY

A fundamental requirement for the use of models in policy is that their predictions be credible. This means that the model must not only get the right answer, but that it must get the right answer for the right reasons. The second point is important, because a model which predicts the correct current concentration of a pollutant because of a cancellation of errors can not be relied upon to provide correct predictions for altered conditions, for example for scenarios of reduced emissions as would typically be required for policy evaluation.

Validation

Full model evaluation and validation should include:

- thorough peer review of the science of the model
- evaluation of the model's ability to predict concentrations of the pollutant of interest, by comparing predictions against measurements, preferably over a wide range of meteorological conditions (this operational evaluation tests the model's ability to get the right answer)
- comparison of the performance of two or more models
- more detailed evaluation of the ability of the model to predict correctly the concentrations of other chemical species involved in the chemical scheme, for example an ozone prediction model would be tested also for its ability to predict the concentrations of NO_x, selected volatile organic compounds and other product species such as PAN (peroxyacetyl nitrate). This procedure, commonly referred to as diagnostic evaluation, tests the ability of the model to get the right result for the right reasons. Diagnostic evaluation also includes, where possible, tests of the individual, component modules of the model.

Model predictions and measurements may be compared at several levels of rigour. The most demanding test occurs when predictions and measurements are paired in time and space. In other words the model is evaluated on its ability to simulate exactly what occurs at a given point at a given time. Less rigorous tests would allow relaxation of the pairing in either time or space.

Relaxation of the time pairing allows a model to score well if it, for example, predicts a similar pattern of ozone concentration through the day, but one hour later than was actually observed. Relaxation of the spatial pairing would allow the model to score well if its predictions for a given point matched well at all times with the measurements made at a different point. Good performance in these relaxed tests might indicate that the chemistry/transport component of the model is performing well, but that there is a deficiency in the meteorological simulation. Thus if the model's wind speeds are too low, high concentrations would reach a given point too late, whereas if the wind direction is off, the prediction will be given for the incorrect place.

Other, more relaxed, tests are also often performed, such as not requiring pairing in either space or time; comparing model predictions averaged over 4 (or more) adjacent grid cells, with point measurements; or comparing various averages. These could be, for example modelled and measured averages over selected areas, or over selected times. Good performance in such tests might suggest that the model will be useful for broad scale, long term applications, but not for the simulation of episodes.

It is important to note that there is a fundamental limitation to how well models can be expected to replicate measurements. This is a consequence of incommensurability, which arises because a model predicts concentrations averaged over a certain volume, whereas measurements are made at a point. For an Eulerian model the volume is the size of the grid cell, which will generally be a minimum of four kilometres on a side, by fifty metres deep, and may well be substantially larger. It is clear that if the concentration of the pollutant in question varies in space, as is almost always the case, the model prediction is likely to diverge from the measurement.

Another concern is that most model validation to date has focused on summer conditions. However, with the increased attention now given to fine particulate matter, which can attain high concentrations at other times of year, more effort will have to be devoted to validation for seasons other than summer.

Model Accuracy

Two main questions must be faced in assessing or discussing model accuracy:

- How accurate is the model?
- How accurate does the model need to be?

These apparently simple questions are, as yet, only partially answerable. In fact, it may never be possible to answer them completely. Further discussion is in order as is considerable further investigation.

How accurate is the model?

For policy purposes it would be desirable to be able to state that the model prediction is uncertain to ± X%. Such a definitive statement can not be made, because model uncertainty depends on many factors, some of them specific to the particular application. Thus, model uncertainty includes contributions from uncertainties in the input data (meteorology, emissions, etc.) and in the model itself. Model uncertainties include uncertainty in parameters like chemical rates, uncertainties in the science on which the model is based, and uncertainties in implementation of the science into numerical form). In addition, the process of model evaluation itself is somewhat uncertain, because of measurement uncertainties, and also because of the problem of incommensurability.

Examples of the results obtained in model evaluation are presented in Table 2. The statistical measures defined in the table are typical of what is used in evaluation, but other measures may also be used.

Table 2. Performance evaluations of models for $PM_{2.5}$ and components with the SCAQA data base in the Los Angeles Basin. Two episodes were used: 24 - 25 June 1987 and 27 - 28 August 1987. (NARSTO, 2003).

MODEL		**UAM-AERO**	**GATOR**	**CIT**	**UAM-AIM**	**SAQM-AERO**
Period		**June 25**	**Aug 27-28**	**Aug 28**	**June 24-25**	**Aug 28**
Statistics		**Normalised statistics[a,b] (%)**	**Normalised statistics[a,c] (%)**	**Normalised statistics[a,d] (%)**	**Normalised statistics[e,f] (%)**	**Normalised statistics[e,g] (%)**
$PM_{2.5}$ mass	error	32	44	46	NA[h]	NA
	bias	+24	-3	+46	NA	10
Sulphate	error	48	28	34	NA	NA
	bias	-10	+4	-30	-21	-33
Nitrate	error	18	68	61	NA	NA
	bias	+11	-21	+47	+52	-14
EC[i]	error	15	57	50	NA	NA
	bias	-10	+30	+35	NA	NA
OC[j]	error	38	49	40	NA	NA
	bias	-38	-44	+14	NA	+38

[a]Normalised error = $\frac{1}{N}\sum_{i=1}^{N}\left|\frac{P_i - O_i}{O_i}\right|$; normalised bias = $\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{O_i}\right)$; where P_i=prediction, O_i=observation, N=number of samples

[b]Mean over all sites and sampling periods of the normalised errors of sampling-period averaged concentrations
[c]Mean over all sites and hours of the normalised errors of 1-hour averaged concentrations (note that sampling periods exceeded 1 hour)
[d]Mean over all sites of the normalised errors of the 24-hour average concentrations
[e]Normalised bias of means = $\frac{\left(\sum P_i - O_i\right)}{\sum O_i}$

[f]Normalised bias of the means over all sampling periods and sites of the sampling-period average concentrations
[g]Normalised bias of the means over all sites of the 24-hour average concentrations
[h]Not available
[i]Elemental carbon
[j]Organic carbon

The range of statistical measures used, and of the values reported in Table 2 indicate that further development in this area is warranted. Table 3 (from NARSTO, 2003) presents a different view of model reliability, containing a

semiquantitative judgement of the certainty which can be associated with the components of and inputs to a modelling system.

Table 3. Levels of confidence in aspects of model simulations (NARSTO, 2003).

Model Aspect	Confidence Level[a]	Model Aspect	Confidence Level[a]
PM Mass Components		**Gases**	
PM ultrafine	VL	SO_2	H
PM fine	M	NO_x	H
PM coarse	M	NH_3	M
PM Composition		VOC	M
Sulphate	M – H	HNO_3	M
Nitrate	M	O_3	M
Ammonium	M	**Spatial Scale**	
OC[b] primary	L	Continental	L
OC secondary	VL	Regional	M
BC[c]	L	Urban	L – M
Crustal material	L	**Temporal Scale**	
Water	L	Annual	L
Metals, biologicals, peroxides	VL	Seasonal	L
		Episodic	M

[a] H: High, M: Medium, L: Low, VL: Very Low
[b] OC: Organic Carbon
[c] BC: Black Carbon

Even if a statement in the desired form could be made about the model, further uncertainty arises because policy applications require the prediction of some future or unknown state. This future state will involve emission changes, as new facilities are built, or as emissions of existing facilities are controlled, and will also correspond to unknown meteorological conditions, and possibly also to changed surface conditions (e.g., changes in land use).

How accurate does the model need to be?

The general answer is that the model predictions should be good enough that model uncertainty does not affect the decisions that are based on the predictions. At least two situations are possible.

- If an atmospheric model is used to provide concentrations or doses that are then incorporated into dose response models, followed by cost/benefit analyses, it is important to bear in mind the uncertainties involved in each step of the calculation. In particular, since errors usually add in quadrature, a model error which is, say, one third of those of the other two steps will not contribute significantly to the overall error. In this type of approach model predictions that are accurate within a factor of two or three may be perfectly acceptable.

- In the contrasting case, "acceptable" pollutant concentrations (or standards) are set by following a weight of evidence approach. Atmospheric models are then used to determine the extent of control required by emission sources contributing to the pollutant burden. The control decisions usually carry significant cost implications, so that model validity is subjected to intense scrutiny. The diagnostic evaluation of the model is important in this application, because, as discussed above, the model prediction is obtained for conditions outside the range included in the validation. The ability of the model to predict correctly the relative change in concentration for a given change in emissions may actually be more important than its ability to predict the absolute concentration. To illustrate, consider the following simplified example:

The ambient concentration of a specific pollutant is 25 μg m^{-3}, whereas the standard for this pollutant is 20 μg m^{-3}. The required reduction is therefore 20%. When the model is run for current conditions, the predicted concentration is 30 μg m^{-3}. To determine the appropriate emission reductions, the model is run to find what level of emissions will give a predicted concentration of 24 μg m^{-3} (i.e., 30 μg m^{-3} reduced by 20%, thus assuming that the model correctly calculates the per cent reduction for a given emission change). This approach is rigorously accurate if the

atmospheric concentrations are directly proportional to emissions, and there is no background contribution from sources which can not be controlled.

Further work on defining model accuracy is clearly needed. It is relevant to note recent work in Germany under the TFS Model evaluation (Tilmes et al., 1999) which looked at policy questions associated with different regulatory options and attempted to specify model performance features necessary to decide cleanly between the regulatory alternatives. The results of this procedure were termed Model Quality Objectives (MQO), as a parallel to Data Quality Objectives, which are normally specified in advance of measurement campaigns. The MQO developed in the initial work were quite stringent, and none of the models evaluated was able to meet them.

EXAMPLES OF ATMOSPHERIC MODEL USE IN POLICY DEVELOPMENT

Presented below are examples of atmospheric model applications which were involved in, or could be of relevance to policy discussions. Also presented are cautionary examples, which illustrates the need for careful analysis in the application of a model.

Assessment of ozone abatement strategies for the Greater Madrid area

Ozone concentrations in the Greater Madrid area can exceed 100 ppb (200 μg m^{-3}). Public notification is required if the concentration exceeds 90 ppb (180 μg m^{-3}), which is the EU guideline. A modelling analysis was carried out to determine the effectiveness of emission reduction scenarios in reducing peak concentrations (Palacios et al., 2002).

The meteorological model used in this work was the Topographic Vorticity Model (TVM), which provided input for the chemical-transport model, which was based on the CIT model developed at California Institute of Technology. The meteorological model covered an area of 300 by 300 kilometres, with a maximum horizontal resolution of 5 x 5 km. Twenty four vertical layers were considered extending to over 15 km. The chemistry and transport were calculated for an inner domain covering 270 x 200 km, also at 5 km resolution, and having 8 levels, up to 4400 metres.

Two episodes were considered in the analysis. They occurred on 14 July 1992 and 15 July 1995. Wind directions were different for these two episodes, which were considered representative of the conditions which most often result in high ozone conditions in the region. The statement was made that high ozone concentrations in the Greater Madrid area are associated with local emissions, as the area is removed from significant regional sources.

Emission scenarios considered are summarised in Table 4.

Table 4. Emission scenarios for Greater Madrid modelling.

Scenario	Description
1	100% increase in road traffic emissions
2	25% decrease in road traffic emissions
3	50% decrease in road traffic emissions
4	70% decrease in road traffic emissions
5	100% decrease in road traffic emissions
6	25% decrease in total anthropogenic emissions
7	50% decrease in total anthropogenic emissions
8	70% decrease in total anthropogenic emissions
9	25% decrease in total anthropogenic VOC emissions
10	25% decrease in total anthropogenic NO_x emissions
11	No anthropogenic emissions
12	Emissions from 0000 to 0800
13	Emissions from 0900 to 2300

Response to these scenarios was analysed in several ways:

1. *Effect on maximum ozone concentration domain-wide:* Reduction in total anthropogenic emissions was more effective than reduction in vehicular emissions alone (remembering that total anthropogenic emissions include motor vehicles). Indeed, total elimination of vehicular emissions, without reducing other anthropogenic emissions, would not reduce peak ozone concentrations for 14 June 1992 below the 90 ppb guideline value, and close to 100% elimination of vehicle emissions would be required for 15 July 1995.
2. *Effect on total amount of ozone above 60 ppb:* This quantity was used to measure total production of ozone in the domain, since 60 ppb appeared to be a background concentration, produced even when anthropogenic emissions within the domain were totally eliminated. Reduction of total anthropogenic emissions by 70% and total elimination of vehicular emissions produced similar reductions in ozone production, i.e., 32 to 51%. This is consistent with what might be expected from the emission inventory, which indicates that 82% of total NO_x emissions and 59% of total VOC emissions are associated with motor vehicles.
3. *Effect of emission reductions for certain time periods:* Scenarios 12 and 13 address the effect on ozone production of eliminating early morning (prior to 9 a.m.) and daytime (9 a.m. to midnight) emissions. It was found that both make a contribution to ozone formation.
4. *Effect of NO_x versus VOC control:* The effect of separate 25% decreases in NO_x and VOC emissions were investigated. At certain locations and times, reduced NO_x emissions resulted in higher ozone concentrations, which indicates that NO_x scavenging is currently limiting the formation of ozone at these locations. Overall, however, the NO_x reduction led to reduced production of ozone for both episodes. On the other hand, reducing VOC emissions produced reduced ozone for only the 15 July 1995 episode, but had essentially no effect during the 14 July 1992 episode.

This study illustrates the approach which is usually adopted in developing policies for pollutant abatement, i.e., develop a set of emission reduction scenarios, and evaluate their effectiveness using a model or models. In practice, the scenarios will have to take into account practical factors, the most important of which will usually be the cost and availability of emission control equipment. In addition, the study brings out some interesting points which also bear on the use of models in policy development:

- What is the most appropriate measure for the pollutant in question? It is now well established that many or all pollutants of current concern have no threshold concentration below which they may be considered harmless. This would suggest that the most appropriate measure should be total exposure for the affected population. However, standards are usually expressed as short term averages (e.g., one hour) not to be exceeded at any specific location. This tends to focus attention on reducing emissions so as to avoid exceedence of the standard, which may not minimise population exposure.
- What time period should be studied? Modern atmospheric models are costly in terms of set up, actual running, and analysing the results. It is therefore very common, as was done in this study, to investigate one or a very few episodes. As was illustrated here, two similar episodes, as judged on the basis of the underlying dispersion characteristics, gave somewhat different results. Appropriate control is required for all conditions, but conclusions based on a limited number of episodes can not be generalised with any degree of confidence. This will be especially true if overall human exposure is of concern, rather than control of peak pollutant concentration.
- The authors of the study actually modelled each scenario twice, using two different chemical mechanisms. Somewhat different results were obtained under certain circumstances, underlining the importance of model validation.

The impact of urban development on air quality and energy use.

Melbourne, Australia was used in a case study, investigating the effects of alternative urban forms on air quality (Manins, et al., 1998). The population of Melbourne was 3,168,300 in 1991, which was taken as the base year for the study. This population is expected to increase by 500,000 by 2011. The purpose of the study was to set up a number of scenarios for the growth of the city, and evaluate their impact on ambient air quality, greenhouse gas emissions and transport energy use.

The growth scenarios were (Figure 4):

- *Business as Usual* – extrapolation of current patterns into the future, with the additional population assigned to zones within the city in proportion to the 1991 base population of each zone.
- *Compact City* – increased population and density of an inner group of eight suburbs. The population density of these suburbs becomes 300 persons per hectare, well above current densities.
- *Edge City* – increased population, housing densities and employment at selected nodes within the middle ring of the city; increased investment in orbital freeways linking these nodes.
- *Corridor City* – focus of growth along three linear corridors emanating from the Central Business District, supported by upgraded public transit infrastructure along the corridors.
- *Fringe City* – additional growth predominantly on the fringe of the city, with 30% of the new population added to currently open areas on the urban fringe, 60% within the outer ring of the city, and 10% to the middle ring. New manufacturing and service industries were also added to the same zones, in the same proportions.
- *Ultra City* – additional growth primarily in provincial cities within 100 km of the principal city, and linked by high speed rail transport. Seventy percent of the new population is added to the four provincial centres, with the remaining 30% added proportionately to the current city as in the Business as Usual scenario.

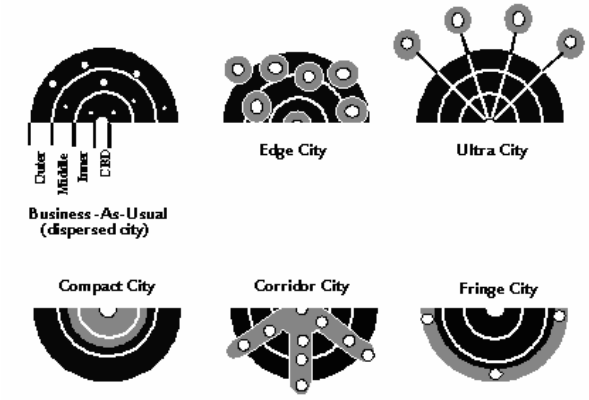

Figure 4: City configurations.

The assessment involved initial application of a land use-transport model (LUTE) which provided emissions for a gridded atmospheric model used to calculate the pollutant concentrations for each scenario.

For the LUTE analysis the region was divided into 26 zones. In each zone emissions were calculated, and gridded, based on the land use of the zone. A transportation gravity model was used to calculate trips between pairs of zones. The trips were assigned to the links between zones, and the emissions calculated, incorporating the effect of congestion on traffic emissions.

The atmospheric model comprised a gridded meteorological model (LADM) driving a chemistry and transport model based on the CalTech model. Computed calculations were combined with population to determine population exposure. To minimise computational and resource requirements the analysis was based on two episodes, one during the winter and the other during the summer. It was clearly understood that a more comprehensive analysis would cover further meteorological conditions.

The results of the analysis may be summarised as follows:

- The Business as Usual scenario is the worst option (with one exception) for all measures (smog and particulate matter exposure, greenhouse gas emissions and transportation energy use).
- The one exception is that the Compact City is worst when exposure to fine particulate matter is considered. This is because considerable use is made of wood burning for space heating in Melbourne in winter time. The corresponding particulate matter emissions are per capita based, which means that the Compact City format concentrates both the emissions and the exposed population. (This conclusion follows even though allowance was made for anticipated tighter control of wood burning emissions by 2011).

- Energy consumption and carbon dioxide emission are closely related, and for both of these the Compact City provided the lowest impact scenario.

Overall the conclusion may be drawn that urban form does affect ambient air quality, and that any type of planning is better than none.

Sensitivity of particulate matter concentration in Ontario to emissions

Although not intended for the development of policy, a recent modelling study carried out in Ontario illustrates the relationship between precursor emissions and ambient concentrations of particulate matter (PM). Atmospheric fine particulate matter is a complex phenomenon, because it may be emitted directly (primary PM), and is also formed by the reaction in the atmosphere of several precursor compounds, including SO_2, NO_x, VOC and ammonia (secondary PM). As is the case for ozone, the possibility of disbenefits also exists, i.e., increased PM concentration when emissions are decreased. A study was therefore carried out to provide a preliminary assessment of the sensitivity of PM concentrations to changes in emissions.

The Models-3/CMAQ system was used with a domain that extended from northern Florida to Hudson Bay, and from west of Chicago to the Canadian Maritime Provinces. Two episodes were considered in this study: one in July 1995 and the other in February 1998. Unlike the case of North American ozone, PM episodes can occur at any time of year. As discussed previously, the conclusions of this study apply rigorously only to these two episodes, but an effort was made to assess how representative the episodes were of high PM episodes in general.

The emission scenarios considered are summarised in Table 5.

Table 5. Emission scenarios for Ontario modelling.

Number	**Reduction**	**Area over which reduction was applied (D - entire domain, C - Canada only)**
1	50% SO_2	D
2	50% SO_2	C
3	45% NO_x	D
4	45% NO_x	C
5	50% primary PM_{10} and $PM_{2.5}$	D
6	50% primary PM_{10} and $PM_{2.5}$	C
7	45% VOC	D
8	45% VOC	C

The chemical composition of the particulate matter is different between the winter and summer episodes, being high in nitrate in the former and high in sulphate in the latter. This means that the precursor dependence is also different, so the two episodes will be discussed separately (Figure 5).

The impacts of the emission changes will differ in different regions of the modelling domain, depending on the spatial relationship between the area considered, the area in which the emissions are affected by the scenario, and the meteorological conditions, especially wind direction. The discussion which follows therefore considers several sub-domains, as defined in Figure 5.

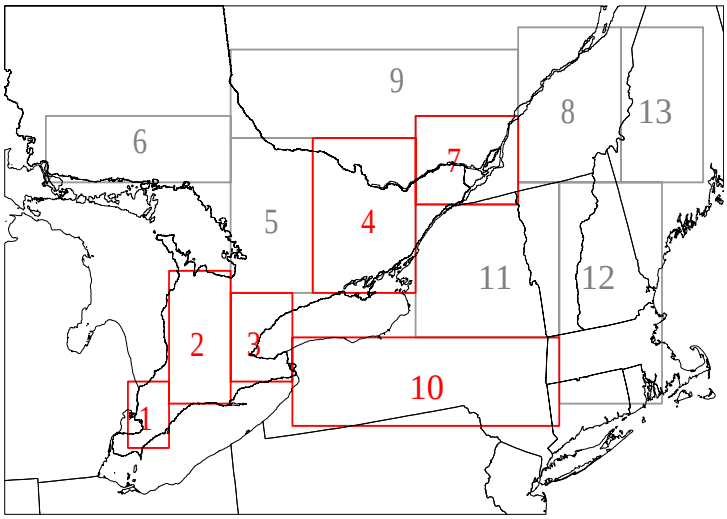

Figure 5: Subregions discussed in scenario modelling.

Summertime Episode

SO_2 reductions:
For this summer episode where the days with high modelled $PM_{2.5}$ were usually dominated by sulphate concentrations, reducing SO_2 by 50% across the domain resulted in 36 to 45% reductions in sulphate, accompanied by small reductions in ammonium and increases in nitrate concentrations. $PM_{2.5}$ reductions were 10 to 32%. Reducing SO_2 by 50% in Canada only resulted in 1 to 15% reductions in sulphate for the sub regions analyzed. The larger improvements were in sub regions 4 and 7, which are downwind of the major urban and industrial centres of Ontario. Reductions in ammonium and increases in nitrate concentrations again occurred. The net changes in $PM_{2.5}$ were reductions of up to 5%.

NO_x reductions:
Reducing NO_x by 45% across the domain resulted in small reductions in sulphate for the sub-regions analyzed. The reductions in nitrate were 26 to 46% with net reductions in $PM_{2.5}$ of 4 to 10%. The response to a 45% reduction in Canadian NO_x emissions was largest in sub regions 3, 4 and 7. For these three regions reductions in nitrate concentrations were in the 20 to 40% range, with corresponding reductions in $PM_{2.5}$ in the 1 to 6% range.

VOC reductions:
Reducing VOC emissions by 45% domain wide resulted in modelled reductions of non-biogenic secondary organic aerosols (SOA) of about 40 to 45%. The net changes in modelled $PM_{2.5}$ were reductions of 1 to 3%. Reducing Canadian VOC emissions by 45% resulted in modelled reductions of non-biogenic SOA ranging from about 2% in southwestern Ontario to 18% in sub region 7. The net changes in modelled $PM_{2.5}$ were reductions of 0 to 3%.

Primary PM reductions:
Reducing primary PM emissions by 50% domain wide resulted in modelled reductions in primary PM concentrations for all size ranges of 50% in all sub regions. The net changes in modelled total $PM_{2.5}$, i.e., primary plus secondary, were reductions of 7 to 19%. Reducing Canadian primary PM emissions by 50% resulted in modelled reductions in primary $PM_{2.5}$ concentrations of about 10% in southwestern Ontario and 25 to 40% in sub regions 3, 4 and 7.

Wintertime Episode

SO_2 reductions:
For the winter episode where the days with high modelled $PM_{2.5}$ were usually dominated by ammonium nitrate concentrations, reducing SO_2 by 50% across the domain resulted in 15 to 33% reductions in sulphate for the sub

regions analyzed. There were small increases in nitrate concentrations and decreases in ammonium concentrations, with net reductions in $PM_{2.5}$ of 1 to 2%.

Reducing SO_2 by 50% for Canada only resulted in 5 to 15% reductions in sulphate for all sub regions except region 10 (New York) where the reductions were smaller. Accompanying changes in nitrate and $PM_{2.5}$ were 1% or less.

NO_x reductions:
Reducing NO_x by 45% across the domain resulted in 6 to 32% reductions in nitrate. There were significant percentage increases in sulphate concentration, but the absolute changes were small. The net changes in $PM_{2.5}$ were reductions of 4 to 17% (but the reduction in sub region 7 was much smaller at 0.4%). Reducing NO_x by 45% in Canada resulted in 4 to 29% reductions in nitrate, again with increases in sulphate concentrations, of about 5 to 20%. The net changes in $PM_{2.5}$ were reductions of 2 to 14%.

VOC reductions:
Reducing VOC emissions by 45% domain wide resulted in modelled reductions of non-biogenic SOA of about 50 to 55%. Because of the small contribution of SOA to total modelled $PM_{2.5}$, reductions were limited to 2 to 8%. Reducing Canadian VOC emissions by 45% resulted in modelled reductions of non-biogenic SOA ranging from 30 to 44%. The net changes in modelled $PM_{2.5}$ were again small, with reductions of 1 to 6%.

Overall, the largest reductions in $PM_{2.5}$ in summertime were achieved by domain-wide reductions in sulphur dioxide emissions. Wintertime $PM_{2.5}$ is dominated by nitrate, and thus responds better to reductions in NO_x emissions.

The sensitivity of predicted PM concentrations to variation in ammonia emissions was also studied. This was necessary, not because control of ammonia emissions is anticipated, but because there are substantial uncertainties associated with the current ammonia inventory. Although the absolute PM mass predicted by the model is affected by the reduction in ammonia imposed in this sensitivity test, it is important to note that the percentage response to the emission reduction scenarios is very similar for the summer time episode. This lack of sensitivity of the response to absolute ammonia emissions gives enhanced confidence in the sensitivities to precursor emissions for the summer. There is somewhat greater variation with ammonia emissions in the winter time, with lower ammonia emissions being associated with lower reductions in PM concentrations when the precursor emissions are reduced. Improvement in the quality of the ammonia emission inventory is clearly required.

Cautionary Tales

To underline the need for care and experience in interpreting model predictions, two cautionary tales are presented below. These were taken from NARSTO (2003).

Kern County California 1985
Modelling results can be quite sensitive to the inputs provided and, in turn, to decisions made to construct those inputs based on available data, however rich or sparse. The experiences associated with modelling efforts conducted in 1985 in preparation for hearings to adopt NO_x emission control requirements for Kern County, California, provide an illustration.

Modelling using UAM-IV was conducted by two groups – state agency staff and a consultant retained by the private sector. Both groups used the same model and the same data base. Each was able to discuss matters with the other if they wished. One group determined that NO_x emissions were limiting in the area of highest O_3 concentrations, the other group that VOCs were limiting, with NO_x reductions having adverse effects on O_3 in some sub-areas. Each recommended that the pollutant found to be limiting in its analysis should be controlled. How could such a difference arise when so much of the two analyses shared the same information and approaches?

Subsequent investigation has uncovered two primary reasons. First, a sub-area in the eastern side of the county was lacking surface meteorological data. It was believed that flow in this sub-area formed a portion of an eddy of considerable size. In order to “give guidance” to the wind field interpolation program, one group inserted a “phantom” meteorological station with prescribed “data”. The other group did not; they instead allowed the

interpolation program to determine the shape of the flow in the area, including those portions in complex terrain. The net result was that each modelling effort produced somewhat different directions for the wind flow passing through the general area where the data were lacking. Since the emission fields were highly variable spatially, this led to mixtures of differing proportions of precursors being transported to the areas of high O_3 concentration.

Second, one VOC surface measurement was available, made in the morning, in a direction generally upwind. To establish initial conditions, one group extrapolated the measurement aloft, in essence setting the concentrations of VOC aloft at levels as high as at the surface. The second group assumed that, since VOC is emitted at the surface, and vertical mixing had yet to occur, VOC concentrations taper off sharply with elevation. Thus the first group specified a high VOC-to-NO_x ratio aloft, the second a much lower ratio. Moreover the group specifying the high VOC-to-NO_x ratio modelled only a relatively short time period; thus, initial conditions displayed an exaggerated impact on O_3 concentrations. The net result was that from two slightly different and reasonable sets of inputs, two very different mixtures of precursors in the relevant downwind area were produced. This, in turn, generated control strategies that were different in kind and not just in degree.

The Pitfalls of Model Simulations with Compensating Errors

Any operational evaluation that is based solely on a simple comparison of observed and model-calculated O_3 concentrations is unlikely to detect existing, compensating model errors. This situation is particularly problematic in the policy context because models having such errors may accurately reproduce a particular observed O_3 field, but for the wrong reasons. This, in turn, can instill a misplaced confidence in a model's predictive capability, possibly leading to inappropriate policy decisions based on its use.

The schematic shown in Figure 6 gives a simplified example of such a situation. It shows an EKMA (Empirical Kinetic Modelling Approach) plot, which is a depiction of the relationship between ozone concentration, shown as contours, and NO_x and VOC concentration. Ozone concentration is a minimum towards the lower left corner, increasing outwards. Here Point A represents the model's predicted O_3 concentration on an EKMA diagram using the actual (or true) NO_x and VOC emission inventories. Point B, on the other hand, represents the model's result obtained with a NO_x inventory that is biased low, combined with a high-biased VOC inventory. By pure coincidence these emission inventories compensate one another to produce the same model-predicted O_3 concentration for simulation B as for A.

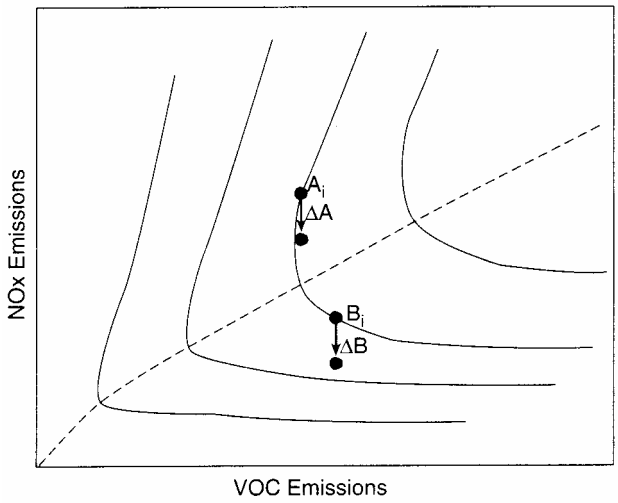

Figure 6: EKMA plot showing contours of ozone concentration as a function of NOx and VOC.

Now consider what happens if these simulations are used to estimate the effect of a hypothetical reduction in NO_x emissions. In the case of the correct emissions the solution moves to the new point on the EKMA diagram indicated by ΔA. As can be seen from the figure, this results in a slight increase in O_3. Conversely, the same NO_x-emission

adjustment to the simulation carried out using the incorrect inventories moves the solution a distance ΔB on the diagram. This corresponds to an O_3 decrease, a directionally incorrect result.

Thus we see that the presence of compensating errors in air quality modelling can pose a major pitfall for policymakers, and could, in principle, lead to the adoption of directionally incorrect control strategies. For these reasons, model applications in the policymaking arena should be carefully screened for compensating errors and related biases. This can be accomplished through rigorous operational evaluations using precursor species as well as O_3 diagnostic testing of modules, independent testing by two or more groups, and comparisons of model results with observations.

CONCLUSION

Atmospheric models constitute the best tools available for the setting of policy, and may, in some cases, be the only tools that are available. This is because the best examples of their kind bring together all current knowledge of pollutant behaviour in the atmosphere, making it possible to unravel the often complex interactions between pollutants and atmospheric dynamics. They also allow the possibility of evaluating hypothetical changes in emissions and other conditions to evaluate potential abatement strategies, or to assess the impact of proposed new emission sources.

However, successful model applications require careful planning and execution. First and foremost is the necessity for understanding the problem, both in terms of the health impacts and the atmospheric science. This includes knowing which pollutant or pollutants are important, and what measure of the pollutants is appropriate. In other words, is there concern about peak concentrations or about longer term average concentrations, or is population exposure a more relevant measure? With the realisation that many pollutants do not have a threshold exposure below which no adverse effects occur, very often comes the need to consider long term average concentrations or exposures. Readers are referred to the Health Effects background paper (Samet and Krewski, this issue) for further discussion of these issues.

Modelling long term effects, as opposed to studying short term episodes, presents difficulties. Apart from the additional input data requirements, running a model for a year takes 30 times as long (in computer time) as it does to run a 12 day episode. When this is compounded over the study of a number of scenarios, the cost quickly becomes prohibitive. Advances have been made in aggregation schemes, which assemble a long-term average from a suitable combination of representative, short-term episodes, but further development is required. It is also relevant to note that while concerns about ozone are mainly confined to the summer months, episodes of high particulate matter concentration can occur at any time of year, necessitating long term simulations.

Clear problem definition amounts to generation of a conceptual model of the situation. A more formal discussion of conceptual models is provided by NARSTO (2003). Based on this conceptual model, the most appropriate mathematical modelling tool can be chosen. Considerations which enter into the choice of model or modelling system include matching the model chemistry to the pollutants of concern, and ensuring that the spatial scale of the model is appropriate. If only one source, or a small group of sources, is important, a Lagrangian formulation may be most appropriate. This is also true if a single receptor, or small group of receptors, is of concern, otherwise an Eulerian model may be a better choice. It is, of course, necessary that the model be properly evaluated and validated, to ensure that the results, and the policies based thereon, are credible.

In fact model evaluation should be a continuous process, since different applications, with different mixes of emissions, meteorological conditions, etc., can lead to differences in performance. Peters et al. (1995) express this viewpoint very strongly, “A model developed or utilized without continual comparison against actual data is less than worthless: it is dangerous.”

Along with the model, an appropriate infrastructure is also essential. This will include all of the appropriate input data, a suitable computing platform, and skilled modellers to carry out the runs, and provide quality assurance and interpretation. These runs will involve scenarios, usually based on altered emissions, but possibly including other changes, such as different treatments of chemistry in the model, or altered meteorological conditions.

Model results will be scrutinised, analysed and interpreted, before being presented to the policymakers. If at all possible the analysis should include incorporation of measurements. Above all, we make a plea for the involvement of all parties – people who make measurements, people who run models, and people who make policy – at all stages of the process. If all of these steps are carried out, the guidance provided by atmospheric models to the policy development process can be used with confidence.

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