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# AIR QUALITY MODELLING AND USER NEEDS

by

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for

# ALBERTA OIL SANDS ENVIRONMENTAL RESEARCH PROGRAM

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#### ABSTRACT

The achievement of satisfactory air quality entails the adoption of one or more air pollution control strategies. Of the four basic strategies available, only air resource management requires the use of air quality models. Atmospheric dispersion models are a subset which can be employed either for fundamental research or for practical decision making. The characteristics of user oriented atmospheric dispersion models are simplicity, clarity, reliability, appropriateness, and practicality. Model performance is determined with reference to accuracy, skill, sensitivity, consistency, generality, integrity, and mechanism. For the successful application of air quality models to the decision process, there must be close co-operation between modellers and users.

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#### 1. INTRODUCTION

#### 1.1 WHAT IS A MODEL?

In general the term "model" may be defined as "a representation of the important properties of any phenomenon". A model cannot have all the properties of the phenomenon, otherwise it would not be a model--it would be the phenomenon itself. A phenomenon that involves the interaction between two or more components is called a system (Hall and Day 1977). A model is an abstraction or simplificiation of a system. The main uses of a model are: (1) describing; (2) predicting; and (3) optimizing.

A model serves to formalize knowledge by integrating observations and theories. If the behavior of a number of parts of a system is fairly well understood, then a model may yield information about the behavior of the complete system that is not obvious from the knowledge of individual parts. A model can generate hypotheses that can be tested against the real world. If there is disagreement in some important attribute then the source of the error must be traced. This leads to careful examination of field data and to explicit statements of assumptions. The interplay of model and empiricism in alternating series is a most powerful scientific tool (Hall and Day 1977).

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A model can predict hypothetical future states of a system or re-construct past states that were not observed. The model goes beyond known circumstances and allows the study of a system under conditions that we are not yet able to observe or create or may never be able or desirous of observing or creating. In other words, models will project the consequences of an action that would be expensive, difficult, or destructive to do with the real system.

Once forecasts are available it then becomes possible to study alternative actions, that is, assess competing scenarios. Certain resources can be allocated in various ways to optimize chosen conditions within the system.

# 1.2 THE CONTEXT OF AIR QUALITY MODELLING

To achieve satisfactory air quality, an air quality manager will employ one or more air pollution control strategies and a variety of air pollution control tactics. An air pollution control strategy is a master plan involving long-term objectives and fundamental principles of action which constitute a basic philosophyor attitude about the means that will be used to reach strategic goals. Air pollution control tactics are the detailed procedures for implementing the strategy, that is, for carrying out the master plan. Tactics will involve short-term objectives and technological expertise.

Four distinctly different air pollution control strategies have been identified (de Nevers et al. 1976):

- 1. Emissions standards: the basic premise is that the amounts of pollutants emitted to the atmosphere should be minimized. Emissions standards may take the form of a numerical rate, a fuel regulation, an equipment design specification, or a complete prohibition. One of the difficulties with this approach is determining the degree of control that should be required. The cost of pollution controls increases at an ever increasing rate, perhaps exponentially, as complete containment is approached. Consequently, the concept of "best practicable technology" has been introduced. "Practicable" implies not only technological feasibility, but also economic, sociology, and political rationality.
- 2. Emission taxes: Each pollutant emitter would be taxed according to some established scale which may be linear (a flat rate of dollars per unit emission) or nonlinear (increasing rate with the magnitude of the emission, like income tax). The scale is set so that the major polluter would find it economical to install pollution controls rather than pay taxes.

It is claimed that the use of such financial incentives will lead to the optimum use of resources. For any given tax structure there will be a breakeven point such that smaller emitters will opt to pay the taxes. This provides a built-in sliding scale that automatically takes care of differences in efficiencies for various sized operations.

- 3. Cost-benefit: The damages due to air pollution and the costs of abatement are first quantified, then only those alternatives that lead to benefits greater than or equal to costs are implemented. Traditionally the quantification takes place by assigning monetary values to all costs and benefits. This is difficult to do in environmental matters where many intangibles must be considered. Roberts and Sievering (1977) introduced a Cost-Risk-Benefit framework that allows an analysis without recourse to complete monetization.
- 4. Air resource management: Ambient air quality standards are the foundation of this approach. Once specified, the amount, location, and time of pollutant emissions are regulated so as to meet those standards.

Each of these strategies is, in fact, a conceptual model of how the actions of environmental managers will affect the behavior of industrial polluters. The adoption of any of these strategies will entail the use of several more models as various tactics are evaluated and implemented. The first three strategies require economic models of varying degrees of complexity. The fourth strategy, air resource management, makes the greatest use of physical and mathematical models.

The four strategies have been briefly described in their 'pure' form. In practice pollution control is usually accomplished by a combination of strategies. Different pollutants or different problems can be approached in different ways. In some instances

elements of one of the alternative strategies may serve as tactics for the primary strategy, or two strategies may be dove-tailed. For example, the Alberta Department of the Environment uses Best Practicable Technology as the primary strategy with Air Resource Management as a supporting strategy.

The term "Air Quality Model" usually refers to a mathematical or physical model used in Air Resource Management. Various aspects of such models will be discussed in this document.

#### 2. MODELS FOR AIR RESOURCE MANAGEMENT

2.1 THE FRAMEWORK

In order to practice air resource management it is necessary to have the following:

- Air quality objectives. These must be in quantitative terms so that the degree of attainment can be measured directly. Thus, they must relate to long or short term concentrations of pollutants rather than to effects of pollution.
- An inventory of emissions. This should include manmade (anthropogenic) and natural emissions (biogenic). Besides total amounts, it is also desirable to have the emission schedule for each source; that is the time variations of the emissions.
- 3. A predictive methodology. This refers to a means of relating air quality to emissions.
- A monitoring system. The data from such a system determine the status of ambient air quality and allow an evaluation of the success of any given tactic or strategy.
- 5. Air pollution control tactics. Alternative actions must be assessed with respect to effectiveness subject to constraints such as technical feasibility, economic viability, and enforceability. Some tactics that may be considered are: land use planning, zoning, tall stacks, flue gas treatment, retrofit equipment, relocation, process change, fuel switching, production cutback, predictive intermittent control, observational intermittent control.
- An enforcement procedure. The air resource manager must have the authority to implement the pollution control plan.

Figure 1 shows the information inputs and their relationships in air resource management.

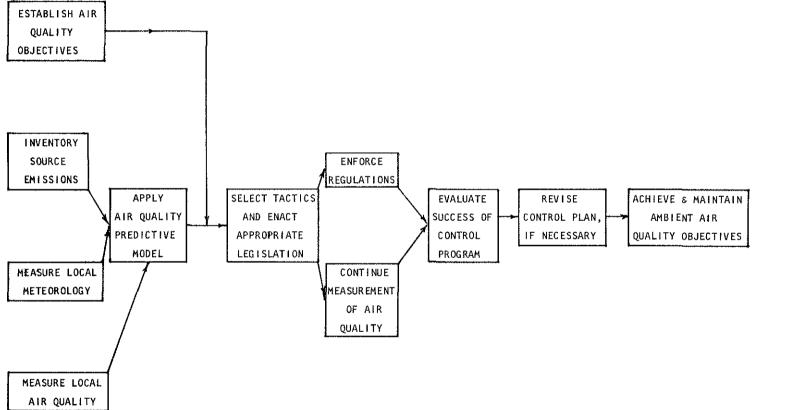


Figure 1. Air resource management requirements.

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#### 2.2 PREDICTIVE METHODOLOGIES

# 2.2.1 Proportional Relations

Called a rollback model in the U.S., the proportional relations model is based on the assumption that the ambient concentration of a pollutant averaged over some appropriate space and time interval is a linear function of the total emissions from that space and time interval. If measured concentrations exceed the air quality objectives, this model leads to a direct computation of the percentage reduction in emissions in the area necessary to achieve the goals. This approach has been widely used in metropolitan areas of the United States because it is simple, understandable and requires little input data. However, it does have serious limitations: (1) it does not account for any of the factors such as source height, source location, meteorology, or topography that cause different sources to contribute differently to groundlevel concentrations at a given point; (2) it is not appropriate for reactive pollutants because of the inherent non-linearities of chemical transformations; (3) it can be difficult to choose the appropriate space and time intervals; (4) it cannot as a practical matter be verified for metropolitan areas; (5) the maximum concentration observed at a monitoring station must be used as if it were the maximum for the entire region of concern; (6) the meteorological conditions encountered during the air quality monitoring period must not differ from those to be encountered at the time of the model projection; (7) the distribution of emissions in space and time must not change over the projection period; (8) background concentrations must remain constant over the projection period; (9) no process affecting pollutant concentrations can be non-linear; (10) rarely is it possible to reduce the emission rate of all sources by the same proportion; and (11) it cannot estimate concentrations from a knowledge of emissions because meteorology does not enter into the technique.

### 2.2.2 Fluid Simulations

The behavior of pollutants with respect to terrain features or buildings can be easily studied by constructing miniature replicas and placing them in a wind tunnel or a water channel. All of the essential variables can be controlled and changed at will. Experiments can be repeated as often as necessary to gather valid statistics or establish reproducibility. There is no waiting on capricious weather systems. The cost of such experiments is considerably less than that of full-scale atmospheric studies.

The biggest difficulty with fluid simulations is that of ensuring that the atmosphere is realistically represented. The scaling or similarity criteria that must be met are not mutually compatible. Consequently, some requirements must be relaxed in order that others may be met. Decisions must be made as to which non-dimensional parameters are dominant and will be matched at the expense of the others. As a result there are always some doubts about the applicability of findings to the real atmosphere.

Neutral atmospheric flows have been modelled with considerable success, but stratified atmospheres still present problems.

# 2.2.3 Empirical Techniques

The detailed analysis of measured concentration data can provide valuable information to the air resource manager. A common approach is the correlation of pollutant concentrations with meteorological conditions and other relevant factors. Statistical methods such as multiple linear regression, principle component analysis, factor analysis, or multiple discriminant analysis can be used to select the variables or combinations of variables which explain most of the variance in the air quality observations.

Moses (1970) described a Tabulation Prediction scheme developed for Chicago's air monitoring network. The concentration frequency distributions for each station were tabulated for various classes of meteorological conditions. Given an existing or forecast meteorological condition, concentrations are "predicted" by looking them up in a set of tables.

Dietzer (1976) obtained a description of the air quality data from a 31 station network using eigenvectors that were functions of space only and eigencoefficients that were functions of time only. By correlating the eigencoefficients with meteorological conditions, it becomes possible to predict the spatial concentration pattern from the meteorological conditions.

Larsen (1969) found that the concentration frequency distribution in a number of U.S. cities could be represented by lognormal distributions with different standard geometric deviations for each city, pollutant and averaging time. Given a measured concentration at a certain averaging time, it was possible to calculate the concentration to be expected at a different averaging time. Stern (1970) proposed the use of the "larrowhead charts," that display frequency distribution as a function of averaging time, for predictive purposes by separating the meteorological effects from the source effects. The frequency distribution that would result from various air pollution control actions could then be synthesized and the action evaluated by the closeness to the match to the objectives.

Barry (1977) demonstrated that the frequency distribution at a monitoring site in the vicinity of a single isolated point source will be exponential for short averaging times. Thus, compliance monitoring of relatively short duration can be used to establish the adequacy of a particular stack design. NULL COMPANY

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Time series analysis has been used by many workers to define the relationship between meteorological variations and pollutant concentrations. Diurnal, synoptic, and seasonal oscillations are readily isolated, for example, Rao et al. (1976), Tilley and McBean (1973).

A variety of statistical approaches are described by Kornreich (1974).

Empirical techniques have not received as much attention as other types of models and the theory is imperfectly developed. To date all such models are strictly valid only for the air quality data set and concurrent conditions from which they have been derived. Generalization has been difficult.

# 2.2.4 Atmospheric Dispersion Models

An atmospheric dispersion model, sometimes called an air quality simulation model, can be defined as a numerical technique or methodology, based upon physical principles, for estimating pollutant concentrations in space and time as a function of the emission distribution and the attendant meteorological and geophysical conditions (after Johnson, Sklarew, and Turner 1976). Put another way, an atmospheric dispersion model is a mathematical method that aims to provide a quantitative cause-effect link between the intensity and spatial distribution of the sources of air pollution and the measured distribution of air quality (Calder 1972).

A clear distinction ought to be made between "models" and "computational algorithms". As defined above a model is a set of mathematical relationships based on physical principles. A computational algorithm is a set of detailed instructions for implementing a model, that is, a computer program or computer code (Roberts 1977). Thus, there can be many algorithms (computer programs) that implement the same basic model. For example, the U.S. Environmental Protection Agency has at least six different variations of Gaussian plume models, two of which, CDM and CRSTER, are familiar to the Alberta Oil Sands Environmental Research Program (AOSERP). Alberta Environment uses three algorithms based on the Gaussian plume model, namely STACKS, FLARES, and PLUMES (Alberta Environment 1978). Given identical input data all algorithms must yield the same results if they are a faithful rendition of the underlying model.

In the turbulent difffusion of material, there are only three basic theoretical approaches (Pasquill 1976). The Taylor statistical theory is related to the Gaussian family of models. The gradient transfer theory is the basis for the K-theory models, often

called simply numerical models. Similarity theory is well developed so far only for the surface boundary layer; consequently it has not been much exploited in air quality modelling. None of the three approaches is universally valid. All have important limitations that must be considered relative to the problems at hand. The U.S. Environmental Protection Agency regards Gaussian models as generally state-of-the-art techniques for estimating the impact of non-reactive pollutants (EPA 1977).

Each of these basic theories has numerous variables that must be assigned values before results are forthcoming. Many of these variables can be modelled in terms of other variables; hence the proliferation of different models in the pages of scientific journals and research reports. Most such models would be impossible to handle other than by computer. The term "computer model" is appropriate in such circumstances. Most models discussed in the literature today fall into this category.

# 2.3 THE ROLE OF ATMOSPHERIC DISPERSION MODELS

Atmospheric dispersion models serve two very different purposes (Stern 1970; Hanna 1973):

1. Fundamental research: Models serve to test our understanding of the physical and chemical processes involved in air pollution. If we cannot model a system, then we do not understand it. In the past, scientists tended to say that they understood the phenomena, back lacked the computational and statistical capabilities to solve the understanding problems. Now, the situation is reversed; enormous computer power is available, but scientists are finding that they lack the physical knowledge to exploit if fully. A research-grade model serves to test ideas by providing detailed representations of the phenomena under study.

2. Practical applications: A decision maker routinely faces a host of questions to which reasonable answers must be given quickly. Applications-grade models allow the exploration of hypothetical situations and their consequences for air quality. Quantitative answers to "what if" questions facilitate the evaluation and assessment of air pollution control tactics and, to some extent, of air pollution control strategies. Model results provide the foundation for decisions that govern many day-to-day activities. Such models are tools which decision makers employ to obtain some of the many information inputs that enter into their deliberations.

#### 3. USER CONSIDERATIONS

A "user" of a computer model is a decision maker whose actions will be affected by the model results. Despite the demonstrated uses (see Rote 1976), potential benefits and the proliferation of available computer models, not all decision makers may be regarded as "users". The Holcomb Research Institute (1978) identified four major factors that influenced the acceptance of computer models by decision-makers:

- Limited resources: Time, money, and personnel are generally scarce and their allocation affects the implementation of programs and policies.
- Political pressure: The power structure and the conflicting viewpoints of different special interest groups must somehow be accommodated.
- 3. Problem complexity: Solutions to one set of problems regularly create unmanageable new problems.

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 Unfamiliarity: There is considerable professional risk in a methodology that is new and often unproven.

Once computer models have been accepted as decision-making tools, it becomes necessary to determine what is required of a model. This is not an easy task for a decision maker. Generally his training, experience, perspectives, goals, methodologies, values, and reward systems will be quite dissimilar from those of a modeller. The great differences often pose a barrier to communication and effective interaction. In such circumstances, an intermediary who is conversant with both technical modelling matters and the pragmatic realities of decision making can be called upon. Such a "policy analyst" has the capacity to translate the goals and constraints of decision making into tangible modelling specifications.

A systematic approach to the evaluation of alternative computer models has been prepared by the staff of Argonne National Laboratory (Rote et al. 1977). The methodology combines technical, importance and pragmatic ratings to arrive at a final comparative judgement as to which of two or more models best suits the application.

The characteristics of user oriented models are described in the following sections.

#### 3.1 SIMPLICITY

The principle of simplicity has always guided physical scientists in their quest for explanations of natural phenomena. This same principle applies in the consideration of competing models for practical decision making. A user will choose the simplest possible model that meets the performance specifications.

Many atmospheric scientists today speak disdainfully of "simple" models and express a clear preference for more "sophisticated" models. Gifford (1973) pointed out that "simple" is not the opposite of "sophisticated" but rather of "complex". The antonym of "sophisticated" is "naive". Simple models are not necessarily naive and may in fact represent the essence of sophistication (Gifford and Hanna 1975). Complex models are not necessarily tied to any deep understanding of physical and chemical processes, and hence can be naive. Hanna (1971; 1973) and Gifford and Hanna (1971; 1973) have demonstrated that simple urban air pollution models estimate observed conditions at least as well as more complex models. In fact, Hanna (1973) noted that, after 10 years of development of more complex models, there was little indication of improved forecasting ability.

#### 3.2 CLARITY

The user of an air quality model needs to understand the components of the "tool" he is using. He should know, in general terms, how the model works, what its limitations are, where problems may arise, and what to do before calling in the specialist, that is, the modeller. It is not intellectually satisfying to rely upon a mysterious "oracle" or "black box" about which nothing can be comprehended. Only if the user is comfortable with the general concepts and terminology--if he feels that he understands the model--will he have confidence in the results. Clarity is related to simplicity only to the extent that a simple model can probably be explained more easily than a complex model. However, even complex models can be explained adequately if enough care and attention are directed towards the documentation. Too often modellers write their documentation for other modellers, with all the emphasis on theoretical and numerical aspects. Even the informed user may find such detail next to unintelligible. This inevitably leads to a wholesale rejection of modelling.

#### 3.3 RELIABILITY

Estimates or predictions of any type must be accompanied by confidence limits if logical decisions are to be rendered. The accuracy of a model is determined by verification, a subject that will be discussed later in this paper. Only when model results can be trusted within known tolerances will a user feel comfortable in applying that model as a problem-solving tool.

It is also important to know how variations in the input data affect the model output. This will inform the user as to the quality of data that will be required and caution him in the event that data of that quality are not available. .....

Model developers rarely have been able to amass adequate data bases designed specifically to test their specific models. Most have merely used whatever was available to them, data bases which are, by and large, hopelessly inadequate owing to small size, limited conditions of measurement, poor quality, absence of measurements of important variables, and other factors. Too often model developers have resorted to comparison with other models and have never tested their models against the real world. To the user such a practice is unthinkable. It has now been recognized that there is a need for more complete data bases which can be used to test a wide variety of models (Stanford Research Institute 1972).

## 3.4 APPROPRIATENESS

The time, space, information, and resource scales of a computer model ought to be appropriate to the problem at hand. A computer model suited to one purpose will not necessarily be suited to a second purpose even on the part of the same user. Different applications will entail different performance goals, different levels of accuracy, different inputs, and different outputs. No one computer model can serve all purposes equally well. Of necessity a decision maker will require a number of computer models, each optimally suited to a particular function. Like a craftsman, the decision maker must have the right tool for the job. Otherwise he may be guilty of the proverbial "killing a fly with a sledge hammer"!

Model developers need to specify the limitations of their models so that they are not used out of context. Ideally, a model would be designed and tailored to the requirements of the user. Often, however, existing research grade models are merely converted into a working format. There are many difficulties with such conversions ranging from inefficiency to site specific restrictions.

#### 3.5 PRACTICABILITY

Resource constraints are very real and must always be kept in mind when developing or adapting a computer model. The following questions must be asked:

- 1. What size computer installation is to be used?
- 2. What are the qualifications of the staff who will be operating the program?
- 3. Are the requisite data readily available?
- 4. Can runs be set up and executed within a reasonable period of time?
- 5. Is the output in the most appropriate format? and

6. Are diagnostic tests available?

Unsatisfactory answers to any of these questions will probably result in rejection of the computer model. Research-grade models almost

always fail in this regard because they tend to take too much computer time, have exorbitant data requirements, produce reams of irrelevant output, and demand the attention of several system's analysts and programmers.

#### MODEL PERFORMANCE

4.

Perhaps the greatest single barrier to extensive model use has been a general lack of confidence in their capabilities. This is due, in part, to the fact that detailed knowledge about many of the basic meteorological and chemical process operating on pollutants in the lower atmosphere is still incomplete. However, perhaps equally as important is the fact that few models have been adequately evaluated and verified. This, in turn, has resulted from both the paucity of suitable data and the absence of performance goals to serve as validation standards. Setting such goals is not easy because they must of necessity reflect the intendeduse of the model and the capabilities of the user. A number of trade-off's or compromises are usually involved in the interests of cost effectiveness (Johnson 1972; Johnson et al. 1976).

In the absence of an appropriate data base, many modellers have simply compared model calculations with observed pollutant concentrations. Unmeasured variables or empirical "constants" are then adjusted to provide the best overall agreement. Such a procedure is a calibration and does not contribute to general confidence in the model. It is entirely possible that the model may have several defective but compensating elements which together yield results that are fortuitously in agreement with observations.

In contrast, a true verification program must involve the careful appraisal and confirmation of individual model elements on the principle that the whole cannot be better than the weakest part.

One or more submodels will typically be used to estimate detailed input from the available gross data. This may involve objective analysis of a field of discrete data points, interpolation between observations in space and time, extrapolation beyond measurement limitations or estimation of values for variables not directly

observed. In many instances such submodels require the modelling of processes not well understood, an inherent weakness in the air quality simulator. To verify such submodels special direct measurements of suitable scale are needed for each variable estimated or converted.

Most of the submodels are mathematical descriptions of the physical and chemical processes that affect air quality. The main formulations are: (1) emissions; (2) transport and diffusion; (3) chemical transformation; and (4) removal mechanisms. Verification of these submodels is accomplished through special experiments designed to isolate and yield information about the particular phenomenon being simulated.

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Air quality modellers with a meteorological background often fail to recognize the importance of the emissions submodel, which is probably the weakest of all the submodels. Hourly source strengths in urban areas are typically known to about ±50% (Hanna 1973). This imposes a severe limitation on the accuracy of air quality predictions even if the diffusion and transport submodels are perfect. Point source submodelling is potentially more reliable because individual stacks can be sampled regularly and continuous stack emission monitors are now becoming commonplace. With area sources, line sources or large numbers of small point sources, verification of the emission submodel is extremely difficult and expensive. This problem has forced some modellers into a calibration procedure designed to remove the variance caused by unknown source conditions.

While the terms validation and verification are often used synonymously, there is a subtle difference which has important ramifications. "Verification" refers to establishing or proving the correctness of the model by rigorous scientific methods. "Validation" implies the formal approval or official acceptance of the model. Thus, validation goes beyond verification and takes into account performance goals and user applications.

The concepts involved in model performance are discussed in the following sections.

### 4.1 ACCURACY

Accuracy refers to the deviation of a model's predicted value from the value actually measured in the field. The agreement between observations and predictions can be expressed by means of various statistics such as mean error, correlation coefficient, or contingency table, to list only a few.

Besides correctness of predicted magnitudes, an air quality model may also need to be capable of predicting hour-tohour variations (Hanna 1973).

For some applications it may be necessary to predict the frequency distribution of pollutant concentrations.

Objective measures of agreement between predictions and observations ought to be used when evaluating different models for accuracy in any of these three areas.

#### 4.2 SKILL

Skill refers to the relative success of a model. Measures of accuracy by themselves have little meaning. To interpret the results of a verification there must be some standard for comparison. Simple models usually provide such standards. In statistics, tests of significance are really nothing more than comparisons with chance, randomness being one of the simplest statistical models. In weather forecasting, skill is often judged relative to persistence in the short term and to climatology in the long term.

In air quality modelling no clear standards have yet emerged although box models have been suggested for the urban modelling standards (Gifford and Hanna 1975) and Gaussian models are generally recognized as state-of-the-art for the diffusion of non-reactive pollutants from point sources (Roberts 1977; EPA 1977). The usefulness of any complex model will depend entirely upon its ability to predict better than any given simple model. If a complex model cannot estimate observed conditions better than some simple model, then in a practical sense it shows no skill. In such a case, the development of complex models for applied purposes is not only unnecessary but unprofitable (Gifford and Hanna 1975).

Also of relevance here is the issue of predictability of the atmosphere both in principle and in practice. Stern (1970) noted that computers had gained a generation on air quality modellers and he warned that "it gains us naught to apply better programming to inadequate physical input data and inadequate physical concepts". Hanna (1973) observed that after a decade of air quality model development there was little indication of improved forecasting ability. Gifford (1976) commented that, while we are on the threshold of basic new insights into theoretical aspects of the turbulence problem, little progress can be expected in practical diffusion modelling. Ramage (1976; 1978) expressed concern that, despite better observations, faster communications, and greater computer power, over the last 10 years weather forecasts have not improved. Robinson (1971; 1971; 1978), Lorenz (1969), and Leith (1971) have indicated that there are fundamental uncertainties that limit the predictability of the atmosphere. Nevertheless, many people believe that a major, dramatic improvement in forecasting is imminent, and this belief is firmly entrenched in official statements and national government policy.

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## 4.3 SENSITIVITY

Sensitivity refers to the magnitude of change in a predicted value that occurs as a result of an incremental change in an input value. Sensitivity analysis of a model determines the expected error and uncertainty in predicted quantities due to error and uncertainty in input parameters. Random errors will be present in all observations and knowledge of model sensitivity will essentially define the accuracies required of various measurements. Systematic errors are most likely to be present when input parameters are

estimated. The magnitude of the variations introduced will indicate whether or not effort must be expended to correct the estimation procedure.

Sensitivity analysis obviously needs to be done prior to the design of any field studies. Each submodel needs to be evaluated separately and as one component of the complete air quality model. This will isolate the key model elements and provide guidance as to the allocation of resources for field verification. Special attention can be focused upon conditions that stress the model, that is, combinations of variables to which the model is very sensitive as these may reveal a basic flaw or shortcoming in the formulations.

# 4.4 CONSISTENCY

Consistency refers to the interrelationship between various submodels. If certain assumptions are made in one submodel, they should not be violated in another. Internal consistency is necessary if a model is to be realistic, that is, if it is to be based on the physics and chemistry of the phenomena rather than in some fortuitous combination of conflicting formulations.

Ideally, consistency also requires that the level of sophistication of each submodel be comparable and that the complexity of each submodel match the physical concepts and physical inputs involved. In practice, discrepancies must be allowed, but satisfactory tradeoffs can often be made after examining sensitivities.

# 4.5 GENERALITY

Generality refers to the range of applicability of the model. The underlying assumptions, both explicit and implicit, of a model will place certain limitations upon the situations in which the model can be expected to perform well. These restrictions may be expressed in terms of time scale, space scale, climatic type, terrain features, or source characteristics. A proper verification will examine all conditions to which the model is expected to apply and perhaps some to which, in principle, it does not apply. Often a verification is done for only one small set of possible conditions. This may provide confidence in the model's use for those particular conditions but lends no support to the potential for more general usage of the model. It is especially important to test models under those conditions that may reveal hidden flaws or shortcomings.

# 4.6 INTEGRITY

Integrity refers to the quality of the data used in a model verification. Assurances need to be provided that the data are sufficiently precise, accurate, repeatable, and generally trustworthy to allow a proper verification to be performed. Care in the acquisition of the measurements is only the first step. Hypotheses which address the data base itself ought to be formulated and tested (Rote 1976). It must be clearly demonstrated that a particular data base is, in fact, adequate for the verification of any given model. If this step is ignored the verification effort will be inconclusive. The modeller will tend to blame the data for the model's poor performance whereas the user is apt to reject the model. If good agreement is obtained it may only be accidental and ought not be considered supportive of model reliability.

This is closely related to maximum utilization of a data set. Most researchers fail to extract more than a small portion of the wealth of information contained in a data set. Much of the knowledge present could be revealed by data analysis techniques quite removed from the air quality model for which the data may have been gathered in the first place. While helping to establish data integrity, such procedures are also cost effective since large sums of money are often expended to obtain these data.

# 4.7 MECHANISM

Mechanism refers to the extent to which the physics and chemistry of the phenomena are embodied in the model, as opposed to statistical summaries or tabular data. This is really nothing more than the distinction between cause-effect relationships and variance

reduction relationships. It is generally accepted that equations expressing causality are superior to those that merely describe a connection between two variables. At present it is not possible to model atmospheric systems entirely with mechanistic equations. Invariably field data which are not well understood must be used in various model components. Models differ in the degree to which this is the case.

# 5. CONCLUSION

The interaction between the decision process and the air environment may include as an intermediate step the activity of air quality modelling. This relationship is shown schematically in Figure 2. Also shown are the links with fundamental scientific research and practical applications, or policy analysis. As the diagram indicates, modelling for applications will reflect the decision maker's perspective whereas modelling for research will focus upon basic knowledge and understanding of the air environment.

After examining the United States experience with environmental modelling and decision making, the Holcomb Research Institute (1978) concluded that:

> Modelling undertaken in an application-oriented, integrative context (i.e., the synthesis and integration of current knowledge) has a better chance of facilitating decision making than modelling undertaken as basic research. This is not to belittle the role of basic scientific research, but to suggest that modelling applied to environmental management must be undertaken with different and perhaps more pragmatic objectives.

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The differences between research and applications are also displayed in the attitudes of atmospheric scientists. Tucker (1976) described the two archetypes and the working associations between them. He concluded that the most effective association involves continuous interaction and discussion such that fundamental research is kept relevant, new ideas can enter operational development without delay, and feedback can suggest new lines of research. In order to establish this he recommended that:

> A mutual recognition is necessary of the need for two types of scientists with different attitudes to tackle different jobs of similar importance ... The gap between these must be bridged, but not narrowed, in such a way that an interchange and flow-on can occur without neutralizing the effectiveness of either.

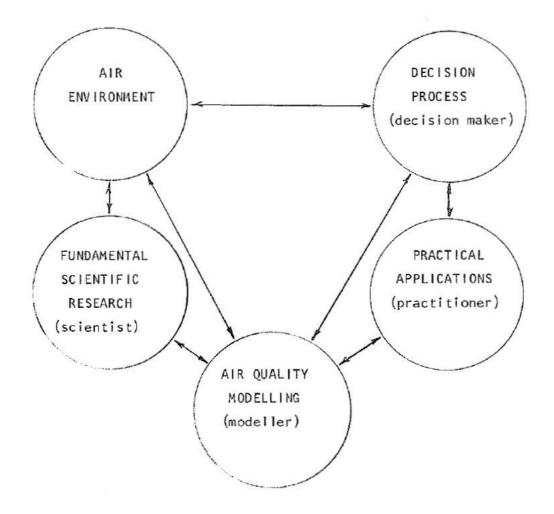


Figure 2. The air environment and interrelationships with various activities (after Holcomb Research Institute, 1978):

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Air quality modelling is potentially of great use in the decision process that directs and controls man's impacts upon the air environment. For that potential to be realized, the modelling activity must address the needs of the decision maker. Hence, the model user should be directly involved in each stage of model development. Before undertaking any model development, the modeller and user should agree as to the objectives of the project and as to its scope in terms of available resources. Performance goals and documentation standards should also be established. To work in other than a fully co-operative manner squanders human resources and imperils the attainment of our clean air objective.

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