REVIEW OF REQUIREMENTS FOR AIR QUALITY SIMULATION MODELS

by

D.S. DAVISON

R.B. LANTZ

INTERA Environmental Consultants Ltd.

for

ALBERTA OIL SANDS

ENVIRONMENTAL RESEARCH PROGRAM

Project AS 4.2.4

September 1980

TABLE OF CONTENTS

		Page
DECLARATION		ii
LETTER OF TRANSMITTAL		iii
DESCRIPTIVE SUMMARY		iv
LIST OF TABLES		xi
ABSTRACT		xiii
ACKNOWLEDGEMENTS		xv
1.	INTRODUCTION	1
1.1	Objectives of this Study	1
1.2	Outline of the Approach to the Model Selection Procedure	1
1.3	Structure of this Report	4
2.	IDENTIFICATION OF USER NEEDS FOR AIR QUALITY MODELS	5
2.1	The Role of Air Quality Models	5
2.2	Discussion of Model Applications in the AOSERP Region	5
2.2.1	Pollutant Characteristics	5
2.2.2	Time Scales	9
2.2.3	Source Characteristics	9
2.2.4	Geographic Features/Topography	9
2.2.5	Spatial Scales	10
2.2.6	Model Output Usage	11
2.3	Definition of User Needs	12
2.3.1	Groups of Users	12
2.3.2	Identified User Needs	12
3.	MODEL TYPES	17
3.1	Models Without Deterministic Dispersion Formulations	17
3.1.1	Rollback Models	17
3.1.2	Statistical Models	20
3.1.3	Box Models	20
3.2	Flow Field Formulations	21
3.2.1	Simple Input Wind Fields	21
3.2.2	Interpolation Wind Fields	22
3.2.3	Potential Flow Type Wind Fields	23
3.2.4	Momentum Conservation Models	25
3.2.5	Momentum and Energy Conservation Models	26

TABLE OF CONTENTS (Continued)

		Page
3.3	Dispersion Formulations	27
3.3.1	Gaussian Dispersion Formulations	27
3.3.2	Numerical Solutions of the Advective-Diffusion Equation	29
3.3.2.1	Discussion of the Eddy Diffusivity Approach	29
3.3.2.2	Eulerian Solution Techniques	31
3.3.2.3	Lagrangian Techniques	32
3.3.2.4	Particle-In-Cell Approach	33
4.	APPLICABILITY OF MODEL TYPES FOR THE SIMULATION OF VARIOUS PHYSICAL PROCESSES	35
4.1	The Role of the Applicability Parameters	35
4.2	Selection of the Relevant Physical Processes	35
4.3	Assignment of the Applicability Parameters	37
4.3.1	Wind Speed and Flow Model Type	39
4.3.2	Wind Direction and Flow Model Type	39
4.3.3	Topography and Flow Model Type	39
4.3.4	Wind Speed and Dispersion Types	42
4.3.5	Wind Direction and Dispersion Types	42
4.3.6	Topographic Flows and Dispersion Types	43
4.3.7	Horizontal Mixing and Dispersion Types	43
4.3.8	Vertical Mixing and Dispersion Types	44
4.3.9	Deposition Adaptability and Dispersion Types	44
4.3.10	Air Chemistry, Multiple Species, and Dispersion Types	45
4.3.11	Plume Rise Submodel Interfacing and Dispersion Types	45
4.3.12	Initial and Source-Dominated Stages and Dispersion Types	
4.3.13	Temporal Variations of Flow and Dispersion Characteristics	46
5.	IMPLEMENTATION CONSIDERATIONS FOR MODEL TYPES	47
5.1	Selection of Implementation Considerations	47
5.2	The Assignment of Implementation Parameters to Model Types	47
5.2.1	Input Data for Model Tuning	50
5.2.2	Input Data for Operational Use	50
5.2.3	Computer Requirements	51
5.2.4	Technical Personnel Requirements	51

TABLE OF CONTENTS (CONTINUED)

		Page
6.	RECOMMENDED MODEL TYPES FOR IDENTIFIED USER NEEDS	53
6.1	Procedure for Model Selection	53
6.2	Worst Case Simulations for Regulatory Standards	54
6.2.1	Assignment of Importance Weighting Parameters	54
6.2.1.1	Wind Speed Parameters	54
6.2.1.2	Wind Direction Parameters	57
6.2.1.3	Topographic Flow Parameters	57
6.2.1.4	Horizontal Mixing Parameters	57
6.2.1.5	Vertical Mixing Parameters	57
6.2.1.6	Deposition and Air Chemistry Parameters	57
6.2.1.7	Plume Rise Parameters	58
6.2.1.8	Initial and Source-Dominated Stage Parameters	58
6.2.1.9	Temporal Variation Parameters	58
6.2.2	Selection of Model Types for Flat-Terrain--Regulatory Standards	58
6.2.3	Selection of Model Types for Complex-Terrain--Regulatory Standards	59
6.3	Frequency Distributions with Stratification Parameters	61
6.3.1	Assignment of Importance Weighting Parameters	61
6.3.1.1	Wind Speed Parameters	61
6.3.1.2	Wind Direction Parameters	61
6.3.1.3	Topographic Flow Parameters	62
6.3.1.4	Horizontal Mixing Parameters	62
6.3.1.5	Vertical Mixing Parameters	63
6.3.1.6	Deposition Parameters	63
6.3.1.7	Plume Rise Parameters	63
6.3.1.8	Initial and Source-Dominated Stage Parameters	63
6.3.2	Selection of Model Types for Flat Terrain--Frequency Distributions	64
6.3.3	Selection of Model Types for Complex Terrain--Frequency Distributions	65
6.4	Long-Term Depositions	67
6.4.1	Similarity to Model Requirements for the Frequency Distributions Application	67
6.5	Long-Range Transport	68
6.6	Synthesis of Recommended Model Types	68
6.6.1	Summary of Recommended Models	68
6.6.2	Comments on the Rationale for the Recommended Models	68

TABLE OF CONTENTS (CONCLUDED)

		Page
7.	RECOMMENDED MODEL IMPLEMENTATION PROCEDURES	71
7.1	Gaussian Frequency Distribution Models	71
7.2	Site-Tuned Gaussian Models for Regulatory Standards	71
7.3	Terrain Models....................................	72
7.4	Importance of Terrain Effects.....................	72
7.5	Representative Wind Data..........................	73
8.	CONCLUSIONS.......................................	74
9.	REFERENCES CITED	76
10.	APPENDIX..	80
10.1	Persons Interviewed for this Study................	80
11.	LIST OF AOSERP RESEARCH REPORTS	82

LIST OF TABLES

Page

1. Summary of Air Quality Model Application Following Rote (1976) 6
2. Classification of Model Applications Following USEPA (1978).......... 7
3. Groups of Potential Users of Air Quality Models for AOSERP.......... 13
4. Summary of Identified Air Quality Model Applications and the Groups of Users Potentially Involved 14
5. A Summary of Model Types.......... 18
6. The Application Elements in the USEPA (1978) Workbook for Comparison of Air Quality Models 36
7. Physical Processes and Their Level of Simulation Utilized in the Evaluation of the Flow and Dispersion Model Types.......... 38
8. Assigned Applicability Parameters for Flow and Dispersion Model Types as a Function of the Simulated Physical Processes.......... 40
9. Implementation Parameters Defined by the Levels of Complexity for the Various Areas of Concern in the Implementation Process.......... 48
10. Implementation Parameters for Model Types.......... 49
11. Importance Weighting Parameters for Various Physical Processes for Each of the Identified User Needs.......... 55

ABSTRACT

Air quality models have long been recognized as a valuable tool for the proper management of the air resources of a region. In view of the high costs involved in adapting and operating air quality models, management of the Alberta Oil Sands Environmental Research Program (AOSERP) considered it advisable to update the user survey carried out in February 1977 (Padro 1977) to ensure that selected air quality models would relate to the improved perceptions of model requirements by potential users. The specific objectives of the present study were to define and priorize types of air quality problems by a survey of user requirements and to suggest types of air quality simulation models which will meet identified needs.

The model selection procedure developed for this study involved application, implementation, and importance parameters to characterize the model types. The application parameters assigned to each model type reflected how well the model type simulated various levels of physical processes which determined the wind flow and dispersion from an industrial source. The implementation parameters considered the operational requirements for input data, computers, and technical personnel. Importance parameters evaluated the degree to which the various physical processes were important for a particular identified user need. This model selection methodology ensured a systematic consideration of the many factors involved in choosing a recommended model type.

Interactive discussions were held with a cross-section of potential model users to ensure that users understood the characteristics and accuracy limits of numerical simulations and to ensure that their perceived needs were properly interpreted in terms of required model characteristics. The interviews of potential users led to the identification of five user needs, of which three appeared to be of particular concern to AOSERP. These were:

1. The maintenance of air quality regulatory standards;

2. The generation of frequency distributions of canopy-top pollutant concentrations as functions of biologically important stratification parameters (such as surface moisture, temperature, time of day, etc.); and
3. The long-term dry deposition patterns.

A number of air quality model types were recommended for meeting the identified user needs. In flat terrain, Gaussian models were considered adequate. In complex terrain, modified potential flow type models combined with a k-theory dispersion formulation were recommended. If flow separation phenomena are important, then a model incorporating momentum and, perhaps, energy conservation equations may be required. The rationale for the selection of the above model types in preference to other model types was discussed in the report.

Specific stages of a model implementation program were outlined. These included:

1. The implementation of a Gaussian frequency distribution model of a modified CRSTER form to include site-specific dispersion parameters and biological stratification parameters;
2. The site-tuning of a Gaussian standards model with a consideration of convective effects for tall stacks;
3. The implementation of a modified potential flow terrain model with site-specific dispersion coefficients;
4. The determination of the spatial distribution of the importance of terrain effects in the AOSERP region; and
5. The generation of a representative wind data base for the frequency distribution model.

ACKNOWLEDGEMENTS

To a far greater extent than in most research studies, this user survey and model review depended upon the co-operation of many people. All of the interviewees willingly gave of their time and very often took a particular interest in the project, providing very useful reports and references. In particular, Av Mann, Randy Angle, and Keith Hage provided on-going advice and support. Marc Wride of Intera, Calgary, provided very useful guidance particularly for some of the biological aspects of the study.

This research project AS 4.2.4 was funded by the Alberta Oil Sands Environmental Research Program, a joint Alberta-Canada research program established to fund, direct, and co-ordinate environmental research in the Athabasca Oil Sands area of northeastern Alberta.

1. INTRODUCTION

1.1 OBJECTIVES OF THIS STUDY

Air quality models have long been recognized as a valuable tool for the proper management of the air resources of a region. Many different types of air quality models have been and are continuing to be developed for a wide variety of specific applications. Considerable work has gone into the identification of needs for models for the Alberta Oil Sands Environmental Research Program (AOSERP). In view of the high costs involved in adapting and operating air quality models, AOSERP management considered it advisable to update the user survey carried out in February 1977 (Padro 1977) to ensure that selected air quality models would relate to the improvement perceptions of model requirements by potential users.

The specific objectives of this study were to:

1. Define and priorize types of air quality problems by a survey of user requirements; and
2. Suggest types of air quality simulation models which will meet identified needs.

1.2 OUTLINE OF THE APPROACH TO THE MODEL SELECTION PROCEDURE

The selection of an optimum air quality model clearly must be related to the model's intended use. However, even when a use has been defined, the selection of a model is not straightforward. One of the selection determinants is often whether the person selecting the model is process-oriented or output-oriented. A process-oriented individual might wish to ensure that all the physical processes which determine the concentrations are realistically simulated. An output-oriented individual may treat the model as a "black box" in which all that matters is the output, so that any modelling artifacts are of no concern. The disadvantage with the process-oriented approach is that considerable complexity may be included in the recommended model which is not requirement for the specific application. Correspondingly, the disadvantage with the output-oriented approach is that the model may be applied in situations in which grossly incorrect predictions result due neglect of important processes and for which it is difficult to recognize when the predictions are wrong, why they are wrong, and how to correct them. The objective in the present study was to utilize a procedure which balanced these two approaches. The procedure (outlined below) was output-oriented to the extent that identified user needs determined the model requirements and process-oriented to the extent that the major features of the processes most important in determining the concentrations were simulated as realistically as required, when averaged over the time and space scales specified by the user needs.

There are a variety of procedures that have been used by various groups to select atmospheric dispersion models. A major division is whether or not a systematic rating procedure was adopted. In a recent CPAR Project, part of the Pulp and Paper Pollution Abatement Program [International Environmental Consultants (IEC) 1975], several factors to be considered in the selection procedure for an atmospheric dispersion model were listed; however, other than for some general considerations, IEC concluded that "no precise rules or decision-making algorithm can be prescribed for weighing these factors and making a selection". The model review study prepared by Padro (1977) similarly did not appear to incorporate a systematic methodology for the selection of the model types. In contrast to these two studies are the selection procedures adopted by Lamb et al. (1973) and Rote (1976). The Lamb et al. study was concerned with critically reviewing modelling techniques for the air quality problems associated with motor vehicle transportation. A total of 20 models were systematically compared with a numerical weighting assigned for the level of simulations of a variety of physical processes determining the pollutant concentrations from highway sources. Rote (1976) presented an objective methodology for evaluating an air quality model for specific applications. The details of the methodology have appeared in a workbook (USEPA 1978); although the Appendices needed to implement the methodology are not yet available. In brief the Rote methodology consists of:

1. Classifying the application in terms of source characteristics averaging time, etc., on an application tree; for each branch of the application tree the workbook prescribes a reference model for comparison purposes;
2. A candidate model is compared to the reference model in terms of the level of sophistication (WORSE, SAME, BETTER) in which it handles the important physical processes, called "application elements";
3. Each of these application elements is assigned an importance rating depending upon the branch of the application tree; and
4. The importance ratings are then applied to the level of sophistication ratings to evaluate the technical merit of the model.

Non-technical (e.g., implementation) considerations are left up to the user to evaluate. Although there may be some concern over the details of the approach, the Rote procedure does provide a systematic methodology for model selection.

In the present study, it was decided to approach the problem of model type selection by developing a modification of Rote's methodology. A systematic procedure was considered necessary due to the need to organize many modelling considerations and a variety of user needs in the selection of an optimum model. In addition, it permitted a more objective appraisal of the problem even though the weighting factors involved in the procedure had to be somewhat subjectively assigned. If new or changed user needs emerge in the future, then the adopted model selection methodology should be helpful in assessing the requirements for an optimum or acceptable modelling approach.

The procedure adopted in this study was to first critically examine the needs of the users in terms of which processes had to be simulated properly in a model and which other processes could be treated in a very simple fashion or could be ignored. The various types of air quality models were then evaluated in terms of how well they could simulate various physical processes; this evaluation was quantified in terms of application parameters with a range of 0 to 10. Implementation parameters, which considered computer requirements, technical personnel requirements, and input data requirements, were then assigned to each model type. Finally, a third set of parameters, importance weighting parameters, were assigned to the various physical process as functions of the identified user needs. The model selection procedure for each identified user need then consisted of a synthesis of the application and importance parameters for each physical process combined with the implementation parameters for that model type. A completely straightforward selection technique would have required an evaluation of the relative importance of implementation and applicability considerations. This approach was not considered to be necessary or desirable since the relative importance is highly user-dependent and can be expected to change with time for a single user. The use of the three sets of parameters (applicability, importance, and implementation parameters) did ensure, however, a thorough and systematic evaluation of the many considerations involved in a model selection.

1.3 STRUCTURE OF THIS REPORT

The model selection procedure, outlined in the previous section, leads to a logical organization of this report. First, the requirements of potential model users are discussed. These identified user needs are based on a series of interviews with a representative cross-section of users. The user needs were analyzed in terms of the role for numerical simulations of the air quality problems. Model types were then briefly reviewed outlining some of the major characteristics of each type. Applicability parameters and implementation parameters were assigned to each model type as a function of the various physical processes that may be important in the determination of air quality. Then, recommended model types were determined for each identified user need utilizing the selection procedure outlined above.

2. IDENTIFICATION OF USER NEEDS FOR AIR QUALITY MODELS

2.1 THE ROLE OF AIR QUALITY MODELS

Air quality simulation models have a long history of use, particularly for the maintenance of air quality standards in the design of new sources. A list of typical applications primarily from the viewpoint of a regulatory agency was compiled by Rote (1976) and is shown in Table 1. However, for AOSERP, this list of possible applications may not correspond to identified user needs. In particular, the output of air quality models may be used by a number of groups beyond the regulatory agencies and so Rote's list could be expanded to include, for example, a variety of biologically related applications. For this study, identified user needs were established by means of interviews with a cross-section of users or potential users of air quality models in the AOSERP region. In addition, the experience of air pollution agencies and researchers in other geographic areas was briefly reviewed to aid in the evaluation of important processes and useful modelling responses. A list of the individuals interviewed and their affiliations is given in the Appendix 10.1, together with a short description of the objectives of the interviews.

2.2 DISCUSSION OF MODEL APPLICATIONS IN THE AOSERP REGION

The user needs or model applications need to be analyzed in terms of their characteristics from an air quality modelling viewpoint. A useful starting point is the application classification scheme presented in the USEPA (1978) Workbook and reproduced in Table 2. From discussions with researchers involved in AOSERP, some initial modifications and simplifications of the application classification scheme in Table 2 can be made.

2.2.1 Pollutant Characteristics

From the user survey, primary pollutants were of far greater concern than secondary ones. It was generally considered that

Table 1. Summary of air quality model application following Rote (1976).

1. Historical air quality trend analysis.

2. Characterization of existing air quality in multi-source areas including:

   Spatial, temporal patterns
   Identification of hot spot
   Identification of worst case
   Source culpability
   Separation of anthro and natural causes
   Selection of clean air sites for special developments (e.g., townsite).

3. Air quality impact analysis

   Existing sources
   Changes in source configurations
   Review of impact statements by regulatory authorities.

4. Integration of air quality impact analysis with planning.

5. Long-term air quality control by means of standards.

6. Short-term air quality control (e.g., supplementary control systems).

7. Stack height design.

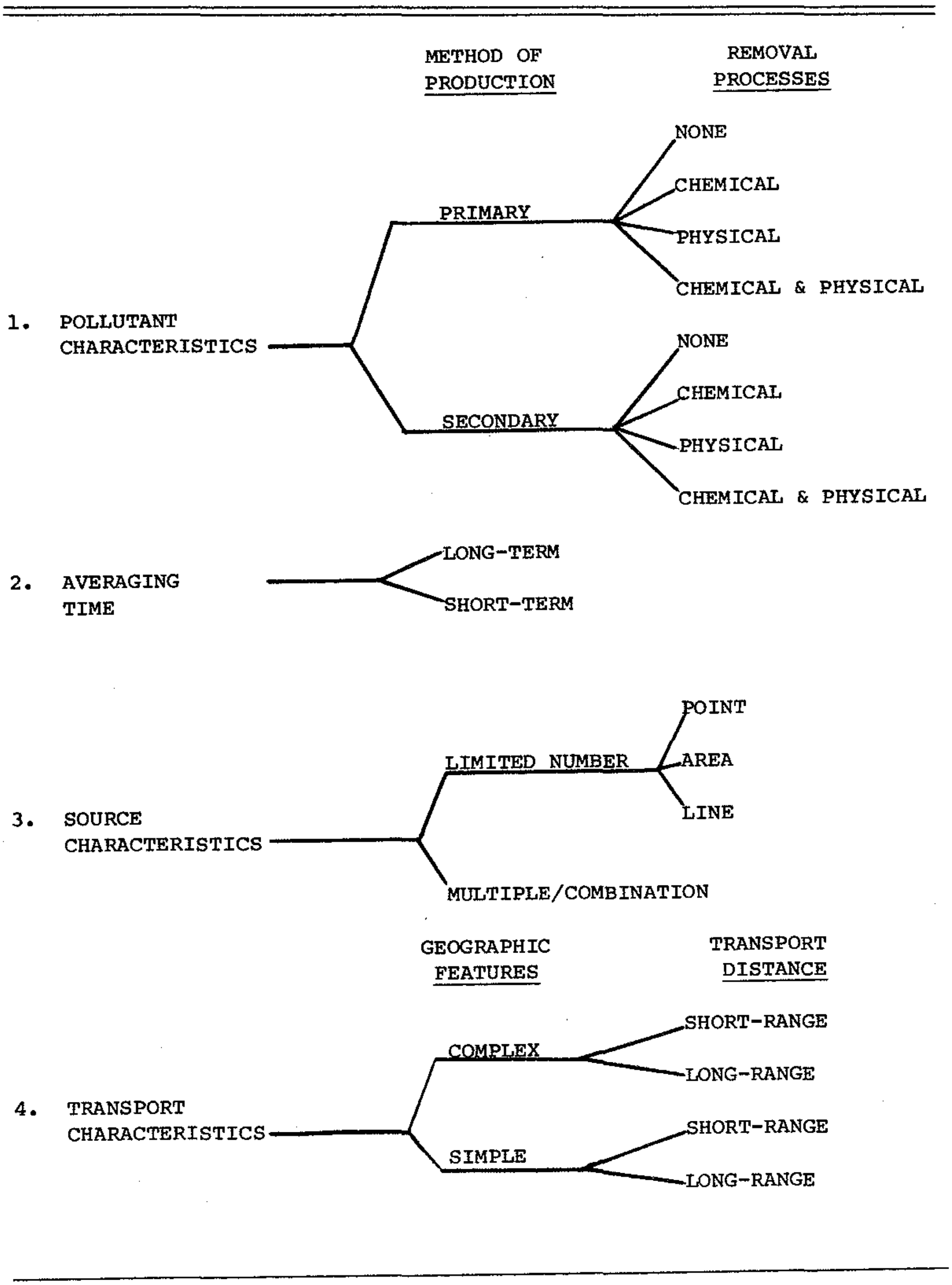
8. Monitoring network design.

9. Emission inventory error diagnosis.

10. Planning new measurement programs.

11. Guidelines for modelling techniques.

Table 2. Classification of model applications following USEPA (1978).



photochemistry and, in fact, all air chemistry would not be of the level of concern that it is in many urban areas. No "exotic" chemistry was believed to be present. Although some oxidation of SO_2 does occur, it was generally believed that this air chemistry did not add significantly to the environmental impact or introduce major new problems. Some concern was expressed that in situ mining processes might release pollutants of a different nature than the surface mining plants and that chemistry might become important in such a situation.

The work of Dr. Barrie at Atmospheric Environment Service (AES) suggested that dry deposition could be decoupled from the air quality model for perhaps 50 km due to the rather small deposition rates. The implication of this decoupling is that even if spatial variations in the deposition rate are large and need to be resolved, these variations of deposition rate can be limited to a deposition model which is independent of the dispersion model and which uses as input the canopy-top concentration values predicted by the dispersion model. Thus the details of the spatial variations of deposition can be neglected in a dispersion model. The air quality dispersion model could perhaps include an average deposition term but this term would not need to be a spatial variable in order to maintain the accuracy of the canopy-top concentrations. There was general agreement among the biologists interviewed that variations of surface moisture, solar insolation, temperature, and other parameters were critically important in assessing the biological impact. However, these stratifications would still not affect how the deposition term is formulated in an air quality model even if different average deposition rates are incorporated for the various moisture/temperature stratifications for the first order estimates of deposition from the air quality model.

Wet deposition has not been well documented to date in the AOSERP region. The presence of convective storms in the summer, when there is the most concern biologically, results in wet deposition of pollutants quite some distance from the source region if the material is entrained into the storm. There has been very little measurable evidence of wet deposition and its inclusion in an air quality model at this time is not considered necessary.

Thus, from Table 2, the pollutants of major concern in the AOSERP region are of primary production and the only removal process that needs to be simulated explicitly in the air quality models is dry deposition and even then, only with a spatially uniform parameter. The qualifiers to the above summary include the possibility of air chemistry being of some concern with the advent of in situ plants.

2.2.2 Time Scales

In Table 2, time scales are limited to short and long averaging times. However, it seems clear that at least two types of time scales are involved for biological users: the resolution time scale (e.g., 1 h) and the time over which these resolution time scales are averaged (e.g., daylight hours). Although a regulatory agency may be primarily concerned with the worst case 1 h or 3 h concentrations, the biological response may be related to the frequency distribution and the joint occurrences of high concentrations.

2.2.3 Source Characteristics

Comparing again with Table 2, the sources of major concern are the principal stacks in each of the oil sands refineries; multiple point sources with definable plume rises and emission rates. Low level fugitive emission may be of some concern in the region close to the plants (less than about 5 km). The urban area source of Fort McMurray and the highway line sources are probably of minor concern to AOSERP.

2.2.4 Geographic Features/Topography

Topographic effects are important for some applications in the AOSERP region but are probably insignificant for other applications.

In the region less than about 10 km from the sources, the main plume centrelines are probably high enough to be largely unaffected by the Athabasca River Valley [recent studies by

Slawson et al. (1979) support this tentative conclusion]. The river valley may affect the local winds measured at Mildred Lake. If the major plumes are high enough to avoid the valley flows, then the adoption of Mildred Lake wind statistics to drive climatological dispersion models may be inappropriate. A careful comparison of Mildred Lake wind statistics with the available pibal and minisonde data base is needed to resolve this uncertainty in terrain effects. The lack of directional dependence of the measured plume sigma values (Davison and Leavitt 1979; Slawson et al. 1979) and the lack of any enhanced turbulence values associated with the river valley at typical plume heights (Davison and Grandia 1978) are further evidence of the lack of major valley effects upon dispersion of the main Great Canadian Oil Sands Ltd. (GCOS)[1] plume and presumably of other similar plumes. However, low-level fugitive emissions are clearly dominated in the GCOS site by the local valley effects.

At greater distances, the presence of several topographic regions within 50 km of the oil sands developments suggests that topographical effects may be important for concentration and deposition patterns at these greater distances. The importance of these topographic variations could be estimated either from concentration data, from monitor stations, or from the results of trial runs by models capable of handling terrain.

The Amoco pilot plant in the Gregoire Lake region is clearly in an area where terrain considerations are important and must be realistically treated in a dispersion model.

2.2.5 Spatial Scales

In Table 2, only short- and long-range transport are considered. From discussions during several interviews, it is suggested that three scales of downwind distance are more appropriate for the AOSERP region. In the region within perhaps 10 km of the sources, the maximum concentrations are usually observed, shear dispersion is probably negligible, and both vertical and lateral dispersion are important. In the region out to about 50 or 100 km,

1. GCOS amalgamated with Sun Oil Company in August 1979, after the writing of this report was completed, to become Suncor, Inc.

lateral dispersion is still important, travel times are still short enough for individual episodes to be considered and for climatological dispersion models to be usefully employed. Beyond about 100 km, only long-term accumulations and averages are of concern. Long-range trajectory models, often working backward from a given receptor, are often employed.

Spatial resolution is another type of spatial scale of concern. Although there may be spatial variations in deposition patterns reflecting different ground cover and moisture conditions, these spatial scales can be decoupled from the air quality model as discussed above. The spatial resolution of the air quality models clearly must be compatible with the spatial variations in the concentrations of concern for each specific user need after allowance for the averaging times of concern. The required model spatial resolution is discussed later for each identified user need.

2.2.6 Model Output Usage

A further classification of model applications not included in Table 2 is the use to which the model output is directed. For a real-time predictive model (e.g., for a supplementary control system), the goal is to minimize the variance of hour-by-hour prediction errors, even though most importance is assigned to the high concentration episodes. In such real-time predictive models, considerable effort may be directed toward the development of predictive tools to describe an evolving boundary layer. In contrast, for regulatory and many biologically related applications, historical data or "worst case" boundary layer configurations can be incorporated. If the application is limited to the maximum concentration in a series of hypothetical worst cases or if predicted concentrations are to be integrated over many realizations, then the accuracy requirements for the boundary layer description are greatly reduced.

2.3 DEFINITION OF USER NEEDS

2.3.1 Groups of Users

The various individuals interviewed to determine identified user needs for AOSERP were treated as representing six groups as shown in Table 3. It is hoped that those individuals interviewed (see Appendix 10.1) were representative of the opinions of the above groups, although it is recognized that not all individuals concerned with the various applications of air quality models in AOSERP were reached.

2.3.2 Identified User Needs

From the discussions during the interviews, it appeared that the various potential applications of air quality models in the AOSERP region could be summarized by five applications. These five applications are shown in Table 4 and are discussed separately in the following paragraphs. The presence of five applications does not necessarily mean that five air quality models are required. Some of the model applications can be treated by the same model as other applications; some applications may require more than one model if, for example, terrain is important only for some particular sites; some applications may not require a response by AOSERP.

The first application in Table 4 is for the types of models incorporated in real-time supplementary control systems. Accuracy on an hour-by-hour basis is important and simulations of the boundary layer development and changes in plume rise are important. Industry is developing models for this application and no direct AOSERP involvement is foreseen.

The second application in Table 4 is for models to be used as tools for the maintenance of air quality standards. These models would be used in a study mode as opposed to a real-time mode and selected boundary layer and plume rise specifications can be input to the models. Accuracy and the ability to handle multiple sources is required. Terrain may be very important for some sites (e.g., Gregoire Lake area) and not so important for other sites, so that more than one model may be optimum. The accuracy requirement means that

Table 3. Groups of potential users of air quality models for AOSERP.

1. Industry
2. Alberta Department of Environment (ADOE)
3. Canadian Forestry Service (CFS)
4. Atmospheric Environment Service (AES)
5. Land use planners
6. Research biologists

Table 4. Summary of identified air quality model applications and the groups of users potentially involved.

Application Numbers	Description of Application	Potential Users
1	Short-term, real-time predictive models for maximum ground level concentrations	Industry
2	Short-term models for maximum ground level concentrations for "worst case" types of simulations for regulatory standards	ADOE Industry
3	Frequency distributions of ground level concentrations with stratification parameters	Research biologists CFS, ADOE Land use planners
4	Long-term deposition and build-up	Research biologists CFS, ADOE
5	Long-range transport and Deposition	AES, Research biologists

Note: The potential users listed in the table are those groups which expressed direct and active interest in the particular applications. Individuals from all groups expressed at least some interest in all of the above applications.

site-calibrated dispersion coefficients are probably required. The specific applications could include the design of new sources, the design and evaluation of monitoring networks, and the assessment of source culpability for specific violation episodes.

The third application in Table 4 is for predictions of frequency distributions of ground level concentrations with appropriate stratification parameters. The stratification parameters might include temperature, surface moisture, solar insolation, season, etc. The importance of these stratifications was emphasized by virtually all of the biologists interviewed; the yearly climatological concentrations are not very meaningful unless broken down into separate populations by the stratification parameters with a frequency distribution of, perhaps, hourly concentrations. The models required for such simulations need to have reasonable lateral and vertical dispersion formulations close to the sources. However, because the model output is integrated over many realizations, simpler boundary layer height and plume rise formulations are probably adequate. The required spatial resolution will depend on the gradient of the hourly concentrations and so will be a function of distance from the sources. Terrain can be expected to be important for some sites. Although the biological effects can be expected to be largest close to the sources, the range of downwind distances of interest is large. The specific applications could include correlation of predicted concentration distributions with biological responses in test sites, the assessment of possible biological impact for planned new sources and the selection of preferred land-use sites for recreation and housing.

The fourth application in Table 4 relates to long-term deposition and build-up. In this application, accumulations of deposited material in the soil, water, snow and biosphere are of concern, rather than direct immediate damage to the biosphere by ground level concentrations of pollutants. A frequency distribution may be important if deposition rates or characteristics of the surface receptor are very different for different seasons, an example being the accumulation of deposited material on the snow during winter with a resultant acid flush in the spring. (This particular concern may not be important due to the buffering of the "brown water" streams in the AOSERP region and the great dilution provided by the Athabasca River.) The output from the air quality model would be used as input to deposition models and soil/biosphere accumulation models and studies. Mean deposition from the air quality model should be adequate with more detailed deposition treatment, if required, coming from decoupled deposition models. The air quality model output is averaged over many realizations and so simplified boundary layer and lateral dispersion formulations may be adequate except possibly, close to the source. The specific applications would include input to studies of long-term future effects with a variety of possible development and emission scenarios.

The final application in Table 4 is for long-range transport models for downwind distances typically greater than 100 km from the source. This application may include both deposition and ground level concentration estimates. However, for such long downwind distances, "narrow plume" trajectory models without lateral dispersion are often incorporated. If a particular sensitive receptor site is of concern, then backtracking trajectories to find the source regions of the air is often done. AES has a continuing developmental program for the long-range transport problem, because they are very often interprovincial and international in nature. Although AOSERP may have concern as to the distant downstream effects, the role of AOSERP in the development or implementation of backward trajectory models does not appear to be clearly defined.

The above sections have identified user needs for air quality models. The associated model characteristics required have been discussed briefly for each user need. The next step is to examine the various types of air quality models and what their inherent characteristics and limitations are. The characteristics and limitations of the model types can then be quantified by means of application and implementation parameters. These parameters can then be combined with importance parameters for the various physical processes as a function of each identified user need to determine the appropriate models for each user need.

3. MODEL TYPES

The large number of air quality simulation models that have been described in the literature can be grouped into a number of model types. Many individual models are minor variations of a basic type often reflecting modifications designed to better simulate a particular physical process.

In many types of models, the formulations for the advective flow field and for the dispersion of the pollutant are decoupled. In these cases, the flow field is first calculated or specified and then the dispersion is superimposed. Thus, in the following discussions of model types, the flow and dispersion formulations are treated separately. Models without a decoupled flow and dispersion formulation usually are relatively simple models without a deterministic dispersion formulation. A summary of model types is presented in Table 5; these model types are discussed in the following sections.

3.1 MODELS WITHOUT DETERMINISTIC DISPERSION FORMULATIONS

The three types of models that do not treat the dispersion processes in a deterministic manner are described in the following sections.

3.1.1 Rollback Models

The simplest form of air quality model is the rollback model. The rollback model assumes that the ambient concentration of a pollutant averaged over appropriate space and time intervals is proportional to the total emission from that time and space interval. It is not an atmospheric transport-diffusion simulation and does not require any meteorological input data.

The simplest proportional formulation for the rollback model is:

$$\frac{C_j - B}{C_o - B} = \frac{Q_j}{Q_o} \tag{1}$$

Table 5. A summary of model types.

1. Non-Deterministic Dispersion Formulations
   - Rollback
   - Statistical
   - Box models

2. Flow Field Formulations
   - Simple input wind fields
   - Interpolation wind fields
   - Potential flow type wind fields
   - Momentum conservation models
   - Momentum and energy conservation models

3. Dispersion Formulations
   - Gaussian
   - Numerical solutions of the advection-diffusion equation
     - Eulerian grid
     - Lagrangian mode
     - Particle-in-cell

where C_j = Concentration indicator in the j^{th} year

C_o = Concentration indicator in the base year

Q_j = Total emission in the j^{th} year

Q_o = Total emission in the base year

B = Background concentration.

Morris and Slater (1974) discussed various types of rollback models and identified four major assumptions implicit in the formulation:

1. The indicator of air quality is representative of the air quality distribution over the region of interest;
2. The distribution of emissions in space and time is relatively stable over the projection period;
3. The meteorological and topographical characteristics of the area are stable over the projection period; and
4. Average background concentration remains constant over the projection period.

Rote (1976) pointed out that the identification of the appropriate time and space scales is non-trivial. The rollback models do not simulate meteorological variations and averaging times must be long. However, the model also cannot handle significant redistribution of the relative source strengths. Any desired reduction of ambient concentrations is non-source-specific. Thus, changes in the source distribution pattern cannot be handled nor can the relative importance of various sources be handled. This consideration suggests that the rollback model is applicable only for single sources or for averaged area sources.

In a modified rollback model (Morris and Slater 1974), the problem of lack of source specificity was approached by expressing the total emissions as a summation from several source categories. A source category "significance weighting factor" was introduced to attempt to relate how much of the ambient concentration was due to each source category. With sufficient emission and ambient concentration data, the relative importance of various source categories could be estimated from such things as ratios of chemical species or isotopic ratios. However, even with modified rollback models, the effects of new sources cannot be predicted, spatial distributions cannot be predicted and long-term averages (of the order of 1 year) are the only appropriate time scales.

3.1.2 Statistical Models

Statistical models are non-deterministic models based on regression analysis of observed concentrations with various stratifying parameters. Statistical models are useful when the sources are constant or when there is a single source and when a large body of data has been accumulated for the regression analysis. An example of such an application is in a supplementary control system where short-range predictions are desired from a statistical model operating with a large data base. Statistical models are generally not useful for planning of new sources or changed distributions of sources. The additions of new sources may invalidate a previously operational statistical model or at least require extensive revision incorporating a deterministic model.

3.1.3 Box Models

In the elementary form, a box surrounds a distributed source such as an urban area. Clean air enters the box from the upwind side, pollution enters from the bottom and instantaneous uniform mixing is assumed. Under steady state conditions, the concentration, C, in the box is

$$C = \frac{Q}{ULH} \tag{2}$$

where Q = emission rate (mass/time)

U = wind speed (mass/time)

L = width of box

h = height of box, usually taken as the top of the mixed layer

A variation of the above simple box model is the moving box model. The moving box model is a simple Lagrangian formulation with smaller boxes over an extended source. The box passes over each area source of strength Q_i in a time interval Δt and so it receives a dose of $\Delta t\, Q_i$ from the i^{th} area source. The concentration in the box is simply the summation of the contributions from each of the area sources. Note that no lateral dispersion is simulated and the moving box model is only applicable where strong lateral gradients in the area sources do not exist. The moving box model (and the simple fixed box model) vertically integrate the concentrations. However, in many (perhaps most) situations, the mixing height may be high enough that uniform mixing is not achieved within the time scale given by the space scale of the source divided by the advection speed (U). Consequently, ground level concentrations for near surface area sources may be grossly underpredicted.

Long-range trajectory models are a particular type of moving box model. Often, an air parcel trajectory is tracked forward or backward in order to identify distant source or receptor locations. Lateral dispersion is often not explicitly formulated. The trajectory models can be useful for correlating specific events at a receptor to a distant source region.

3.2 FLOW FIELD FORMULATIONS

In the discussion of deterministic models, it is helpful to consider separately the advective flow field and the dispersion of the pollutant within that flow field. Since the flow field, in some models, can affect the dispersion formulation, but not vice-versa, it is appropriate to discuss the flow formulation first. Four classes of flow formulation of increasing complexity are discussed below.

3.2.1 Simple Input Wind Fields

The simplest procedure for the specification of the flow field is to simply input a constant wind. Inputing a wind profile in order to abstract an "effective advection speed" in conjunction with a plume rise formulation is of the same type.

Some dispersion models can operate with a wind profile and, in such cases, an input profile in the form of a power law is often utilized.

These first two types of input wind field are routinely used for planning and study purposes. The type of flow input scheme used (mean or profile) depends upon the dispersion formulation. However, complex terrain situations present complications that are seldom handled well by such simple input specifications.

3.2.2 Interpolation Wind Fields

In complex terrain situations, one commonly used technique to determine the flow field is to interpolate from an array of measurement sites. The simplest form of interpolation is to generate a two-component horizontal wind field which may not be divergence-free. However, most models using interpolation wind fields attempt to approximate a divergence-free flow field. In complex terrain, two-component wind fields are sometimes made divergence-free by generating the third component as:

$$W = - \int_0^z \left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} \right) dz \qquad (3)$$

In areas of only slight terrain, vertical velocities are sometimes assumed to be zero. Variational analysis is often used in order to generate an adjusted wind field with a minimum discrepancy from observations subject to the strong constraint that the adjusted field be horizontally divergence-free. An excellent summary of the variational method applied in the flow model, MATHEW (Lawrence-Livermore Labs), is contained in the report by Reid et al. (1978).

Interpolation wind fields have certain limitations regardless of whether there is subsequent processing to generate a divergence-free field. Terrain influences or spatial variations are included only to the extent that they are reflected in the measurements. From fixed anemometers, the routine measurements of vertical velocity are not always available. If a divergence-free wind field is also required, then a choice must be made as to whether to assume a zero vertical velocity as "observed" and use a variational approach or else to generate a vertical velocity field. In regions of significant terrain, the variational approach may be questionable unless better "observed" vertical velocities can be generated. However, generating a vertical velocity field means that the observational errors are directly inserted into the dispersion model.

Interpolation wind fields may generate spurious spatial variations due to the data used to derive them. Statistical sampling problems, particularly for pibal measurements, can introduce substantial errors in the mean wind estimates for single realizations. The acceptability of these sampling errors depends on the application of the model and, in particular, on the amount of averaging of the individual realizations. A discussion of sampling errors for pibals and minisondes was presented by Davison and Leavitt (1979); typical uncertainties in the wind field are 20% with a dependence on the energy in the low frequency part of the spectrum. It is clear that the technique used to generate the interpolation wind field should be designed carefully to ensure that differences between measurement sites reflect real spatial variations in the average winds rather than statistical fluctuations within a single population.

3.2.3 Potential Flow Type Wind Fields

Potential flow solutions can provide an indication of the gross flow characteristics in a region of complex terrain. If the velocity field can be treated as irrotational, then a scalar velocity potential can be defined; that is if:

$$\nabla \times \vec{V} = 0 \tag{4}$$

then

$$\vec{V} = \nabla\phi \tag{5}$$

where ϕ is the velocity potential. For an incompressible fluid, the equation of mass conservation (continuity equation) is:

$$\nabla . \vec{V} = 0 \tag{6}$$

and so applying the velocity potential expression generates Laplace's equation:

$$\nabla^2 \phi = 0 \tag{7}$$

Equation (7) means that the velocity potential for irrotational flow in an incompressible fluid is a solution of Laplace's equation. Laplace's equation can be solved analytically for flow over a variety of shapes and these solutions provide some guidance in regions of complex terrain (see for example Bronwell 1953:276 ff. or Egan 1975).

The limitation of pure potential flow solutions is that the real atmosphere is not irrotational. The solution of Laplace's equation for boundary conditions of constant potential in the vertical direction and no terrain results in horizontal velocities which do not vary with height. In any real boundary layer, there are viscous effects or turbulent effects which make the fluid rotational. Thus, in the surface layer, potential flow theory is invalid.

The adoption of a two layer model is one way of overcoming the problem of rotational flow. Hino (1968) developed such a two-layer model with a potential flow solution in the outer layer and a set of boundary layer equations for the surface layer.

Another way of compensating for rotational flow (Lantz et al. 1972) is to adopt a modified potential flow of the form:

$$\vec{U} = \vec{K}.\nabla\phi \tag{8}$$

where K is a three-component empirical flow coefficient having a power-law dependence up to some reference height and unity above that reference height. The resultant flow fields in non-terrain situations have a power-law profile which can be made stability dependent, topped by a potential flow solution. Application of equation (8) into the mass conservation equation leads to:

$$\nabla . (K.\nabla\phi) = 0 \tag{9}$$

In a terrain situation, the surface boundary condition is that the normal component of velocity be zero and equation (9) is solved numerically.

Although multi-layer models and potential flow models allow a simulation of terrain effects, they do have a number of limitations. There is no allowance for flow separation and recirculation phenomena. There is no explicit allowance for flows due to thermal instabilities including drainage flows and convective flows. However, by adopting stability dependent boundary layer simulations in the multi-layer models and stability dependent flow coefficients in the modified potential model, the variation in the flow field due to ambient stability effects can be simulated.

3.2.4 Momentum Conservation Models

If phenomena such as flow separations are important, then the flow field can be simulated by solutions of the momentum conservation equations (Navier-Stokes equation). In its basic form, this type of model incorporates the momentum conservation equations, the mass conservation equation, and a specification of the density (a form of an equation of state) giving five scalar equations in five unknowns (three velocity components, pressure, and density). For an incompressible, Newtonian fluid, the momentum conservation equation (Navier-Stokes equation of motion) can be written (see for example Batchelor 1967, Chapter 3):

$$\rho \frac{D\vec{U}}{Dt} = \rho\vec{F} - \nabla p + \mu\nabla^2\vec{U} \tag{10}$$

where D/Dt is a material derivative

F are body forces.

The body forces can include gravity and fictitious body forces (centrifugal force, Coriolis force) due to a rotating co-ordinate system.

For a turbulent fluid, the velocity field is often decomposed into mean and fluctuating components. In first-order closure models, the second-order terms generated by substitution of mean and fluctuating velocity components into the Navier-Stokes equation are represented by eddy viscosity coefficients:

$$-\rho \frac{\partial \overline{U_i U_j}}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} = \frac{\partial}{\partial x_j} \mu^T_{ij} \frac{\partial U_i}{\partial x_j} \qquad (11)$$

where $u_i u_j$ = a second-order fluctuating velocity mean correlation for velocity components in the i^{th} and j^{th} direction.

$_{ij}$ = is the equivalent Reynolds stress

$_{ij}$ = is the turbulent eddy viscosity coefficient for the ij - component of the Reynolds stress.

With the closure hypothesis of equation (11), the five scalar equations can be solved numerically with specification of boundary conditions and eddy viscosity coeffients. In many practical situations, the molecular viscosity can be ignored and the body forces represented only by gravity.

3.2.5 Momentum and Energy Conservation Models

The basic formulation involving the momentum and mass conservation equations is sometimes augmented by inclusion of a density formulation rather than a time invariant density specification. Variable density can be simulated by an equation of state which introduces a sixth variable, temperature, and the energy equation which provides the sixth scalar equation. For many applications, the energy equation can be simplified to a thermal energy equation of the form:

$$\rho\, C_p \frac{DT}{Dt} = \lambda \nabla^2 T \qquad (12)$$

where c_p = the specific heat

λ = the thermal diffusion coeffient

Higher order closure models have also been developed for detailed flow specifications. In these models, the second-order correlations are not expressed in terms of gradients of first-order terms as in equation (11); instead, a series of governing equations for the second-order correlations are used (see for example Busch 1973). However, third-order correlations then appear and a closure hypothesis is still required involving third- and second-order correlations. Higher order closure models have been primarily developed for studies of the structure of turbulent boundary layers (e.g., Deardorff 1973; Wyngaard and Cote 1974). The authors are not aware of any applications of second-order closure models to industrial dispersion problems; the complexities and cost of solving typically 18 simultaneous equations at each grid point for each time step may not generate sufficient improvement in the flow field and eventual concentration estimates to warrant their use.

3.3 DISPERSION FORMULATIONS

As discussed above, the dispersion and flow formulations in deterministic models can usefully be considered separately. In the following sections, several dispersion formulations are discussed. Each of these dispersion formulations could conceivably be applied to each of the formulations discussed above.

3.3.1 Gaussian Dispersion Formulations

The diffusion equation has been the starting point of most mathematical approaches and represents a generalization of the classical equation for conduction of heat in a solid. For an incompressible fluid (see for example Pasquill 1974:108 ff.):

$$\frac{\partial \overline{C}}{\partial t} + \overline{U}_i \frac{\partial C}{\partial x_i} = - \frac{\partial \overline{u_i' C'}}{\partial x_i} \qquad (13)$$

where there is summation over the component indices, and where C is concentration and prime quantities are fluctuations about the mean (denoted by an overbar). Using a simple gradient-transfer assumption, often called k-theory assumptions:

$$\frac{\partial}{\partial x}\left(\overline{u'C'}\right) = \frac{\partial}{\partial x}\left(K_x \frac{\partial C}{\partial x}\right) \qquad (14)$$

If the k's are constant, independent of x, y, or z, then the diffusion process is called Fickian. For a steady source with a constant wind speed, U, (equation 13) can be written (see Sutton 1953:134 ff.):

$$\vec{U}\ \frac{\partial C}{\partial x} = K_y \frac{\partial^2 C}{\partial z^2} + K_z \frac{\partial^2 C}{\partial z^2} \qquad (15)$$

Classically, the Gaussian formulation has been viewed as the solution to the steady state advection-diffusion equation with constant diffusion parameters and uniform wind (equation 15). This requires the Gaussian sigmas to be defined by:

$$\sigma_y = \left(\frac{2\ K_y\ X}{\vec{U}}\right)^{1/2} \qquad (16)$$

If the vertical co-ordinate is referenced to the ground rather than the plume centreline, and a reflecting boundary condition is adopted at the surface, than the concentration distribution becomes:

$$C\ (x,\ y,\ Z) = \frac{Q}{2\pi\ \sigma_y\ \sigma_z\ U}\ \cdot$$

$$\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2 - \frac{1}{2}\left(\frac{Z+H}{\sigma_z}\right)^2 - \frac{1}{2}\left(\frac{Z-H}{\sigma_z}\right)^2\right] \qquad (17)$$

where H is the effective source height.

Recently, Gifford (1975) has emphasized that the Gaussian solution is really an empirically based assumption about the form of the concentration distribution. In this approach, the Gaussian solution is not tied to the simplified advection- diffusion equation (15) and the sigmas need not have the $X^{1/2}$ dependence of equation

(16). A detailed review of the various sigma specification schemes has been completed recently by Davison and Leavitt (1979); an optimum sigma specification scheme based on the AOSERP data base was included in that report. The sigmas can also be generated from more advanced types of models. An example of this approach applied to the AOSERP region is the work by Kumar (1978).

For cases of limited mixing, it is common to assume complete reflection at the trapping inversion utilizing the concept of multiple image sources. Pasquill (1976) studied the sensitivity of the calculated concentrations and recommended a multiple image source method with two vertical sources above the mixed layer and two below ground level as providing adequate concentration estimates at all downwind distances.

The Gaussian formulation has been applied in terrain situations with various approximate procedures for estimating the height of the centreline above terrain. These terrain modifications are actually modifications of the flow field within which the Gaussian formulation is applied. These terrain procedures have major technical limitations, especially in three-dimensional terrain.

3.3.2 Numerical Solutions of the Advection-Diffusion Equation

3.3.2.1 Discussion of the eddy diffusivity approach. The advection diffusion equation (13) can be simplified by a gradient-transfer-type assumption equation (14) (the k-theory assumption) to yield an equation that can be solved numerically. The application of the closure hypothesis of equation (14) is inappropriate close to the source, as is seen clearly from Taylor's statistical theory (see for example Pasquill 1976:126). However, at greater downwind distances, the relationship in equation (14) can be valid simply on dimensional grounds. Pasquill (1976) indicates that Taylor's statistical theory can be represented properly at long dispersion times by an "effective eddy diffusivity" of the form:

$$K_i = \overline{U_i'^2} \, t_L \qquad (18)$$

where u'^2_i = the standard deviation of the i^{th} component of the turbulent velocity

t_L = the Lagrangian integral time scale.

The significance of the Lagrangian integral time scale [see Pasquill (1974) or Tennekes and Lumley (1972) for further details on integral scales] is that it determines what constitutes a "long" dispersion time or equivalently a "large" downwind distance. The Lagrangian integral time scales in the AOSERP region were estimated by Davison and Grandia (1978) as typically 100 s based on airborne measurements of the atmospheric turbulence structure. For wind speeds at plume height of 5 to 10 m/s, the corresponding downwind distances are 0.5 to 1 km. Thus a typical "large" downwind distance at which the effective eddy diffusivity concept might be expected to be reasonably applicable is perhaps 2 km.

From an operational point of view, a k-theory model could work even if the gradient-transport hypothesis is questionable so long as the dispersive nature of the turbulence could be specified as a field variable independent of the source. However, it is clear from Taylor's statistical theory that the use of k-theory from small diffusion times could be equivalent to neglecting the additional effects of the small-scale eddies.

Thus, the relative importance of eddy size scales changes as the size of the plume changes and, close to the source, a k-theory model may have serious problems. In many practical problems, however, the region close to the source is the region in which plume buoyancy effects are significant. Thus, for these situations, no passive diffusion formulation is adequate and an initial dilution formulation following, perhaps, Briggs' (1975) approach is required (see Davison and Leavitt 1979).

In an attempt to overcome the near-source limitations of k-theory, Berkowicz and Prahm (1979), Prahm et al. (1979), and Prahm and Berkowicz (1979) have represented the diffusion coefficients in spectral form. This development does appear to overcome the problem of the application of k-theory close to the source. However, as discussed above, the dispersion of industrial buoyant plumes should not be treated as environmentally dominated until typically 1 km downwind. Thus, the spectral diffusivity concept, although very interesting theoretically, may not be particularly useful for the AOSERP region.

3.3.2.2 Eulerian solution techniques. Although the eddy diffusion concept (k-theory) has the limitations outlined above close to the source, it is a widely used formulation in diffusion studies. The most common way of solving the advection-diffusion equation, simplified by k-theory, is to employ finite differencing techniques. The major problem in employing finite differencing is the presence of numerical dispersion effects arising from the advection term. However, if the mean flow is mostly unidirectional ($V = W = 0$), then numerical dispersion is in the direction of advection and, for a steady state solution, the problem is not serious. If numerical dispersion is a problem, then finer grid spacing and smaller time steps may be required.

A variety of solution techniques have been developed to attempt to reduce the numerical dispersion effects. Long and Pepper (1976) studied the numerical dispersive behavior of six numerical schemes in a fluid flow with constant angular velocity. The schemes tested were the following:

1. The donor cell method;
2. The fully implicit method;
3. The Crank-Nicolson method;
4. The cubic spline quasi-Lagrangian method;
5. The linear Chapeau function method; and
6. The Egan-Mahoney second moment method.

Although the test is unrealistic in that such a flow field would not be encountered in atmospheric dispersion problems, it does provide a standardized test for the numerial dispersion effects. The original work should be referenced for specific conclusions and qualifying statements. However, it does appear that the problem of numerical dispersion can be largely rectified with better finite differencing schemes. This conclusion is the same as was reached in a review of Eulerian-grid finite differencing for urban models by Liu and Seinfield (1975).

Another technique to avoid truncation effects is a fractional step technique developed by Runca and Sardie (1974). Numerical dispersion is avoided by separating the advection and dispersion at each time step. By appropriate selection of the grid element sizes and a discretization of the wind profile, the concentration field can be everywhere advected an integral number of grid blocks at each time step. The diffusion is solved by Crank-Nicolson finite differencing. It appears that the technique can be adapted to a fully three-dimensional situation.

A number of spectral techniques (finite elements) have been developed recently in attempts to overcome the numerical dispersion effects arising from the advection term. In a review paper, Bass and Orszag (1976) suggested that full spectral techniques had not yet been successfully formulated for application to the study of a passive scalar in a sheared turbulent velocity field. Christensen and Prahm (1976) presented a pseudospectral model, a variation of the spectral technique, in which only the space derivatives are computed by means of finite Fourier transforms. The local products and time derivatives are evaluated in physical space. They managed to overcome the need for periodic boundary conditions by introducing a boundary damping term and a filter to suppress the resulting aliasing effects. However, it is not clear that the technique is applicable in terrain situations where complex models have major advantages over simpler techniques.

3.3.2.3 Lagrangian techniques. Formulating the model in a Lagrangian co-ordinate system avoids the advection terms in the advection-diffusion equation which present the numerical dispersion problems for

Eulerian grid schemes. In this way, the diffusion equation becomes (see for example Eschenroeder et al. 1972):

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial C_i}{\partial z}\right) + S_i + R_i \qquad (19)$$

where C_i = the concentration of the i_{th} species

S_i = a source term

R_i = a reaction term

This type of formulation is an elaboration of the moving box models discussed earlier to include a better vertical dispersion formulation. However, the model does not allow for horizontal dispersion nor does it allow for converging or diverging wind flows and wind shear. Lagrangian types of models have been found to be useful for urban situations and for large area sources; they do not appear to be particularly useful for a region with a relative small number of major sources such as the AOSERP region.

3.3.2.4 Particle-in-cell approach. Sklarew et al. (1971) introduced a particle-in-cell method which incorporated the dispersion into a fictitious total equivalent transport velocity. Starting from the k-theory form of the advection-diffusion equation, Sklarew introduced turbulent flux velocities, U_{if}, defined by:

$$U_{if}C = - \overline{K_i} \frac{\partial C}{\partial x_i} \qquad (20)$$

The advection-diffusion equation, for a non-divergent mean wind field, becomes:

$$\frac{\partial C}{\partial t} = - \frac{\partial\left(\overline{U}_i + U_{if}\right)C}{\partial x_i} \qquad (21)$$

By defining the term in brackets in the above equation as the total equivalent transport velocity, the equation is seen to be identical in form to the mass conservation equation for a compressible fluid.

The particle-in-cell method simulates equation (21) by introducing a large number of Lagrangian particles into an Eulerian grid and moving each of these particles with the fictitious total equivalent transport velocity at each time step. The appropriate total velocity for each particle is interpolated from the total velocities calculated at each Eulerian grid cell centre. This mixed Lagrangian/Eulerian approach avoids the numerical dispersion problems associated with the direct numerical solution of the advection diffusion equation. The concentration is just the number of particles in an Eulerian cell or alternatively, each particle can be assigned a volume which is distributed proportionately to each Eulerian cell it overlaps. The particle-in-cell method is utilized by several models including the ADPIC model (Lange 1978), which has been studied previously for possible AOSERP applications by Reid et al. (1978). The major problem with it lies in its large computer costs.

4. APPLICABILITY OF MODEL TYPES FOR THE SIMULATION OF VARIOUS PHYSICAL PROCESSES

4.1 THE ROLE OF THE APPLICABILITY PARAMETERS

In this section, the flow and dispersion model types are evaluated in terms of their ability to simulate various physical processes which may be important for the prediction of ground level concentrations. The result of this evaluation is a matrix of applicability parameters. These applicability parameters are combined with importance rating parameters for each identified user need to arrive at a preliminary technical evaluation of the models. However, implementation considerations must also be incorporated before an optimum model type can be recommended.

4.2 SELECTION OF THE RELEVANT PHYSICAL PROCESSES

The selection of the relevant physical processes, by which model types are classified to generate applicability parameters, requires a distinction between choosing a model to be implemented and evaluating a specific application of that model. The core of any atmospheric dispersion model is the technique used to simulate the flow and dispersion. The flow and dispersion types often limit the ability of the model to accurately predict the ground level concentrations and to simulate other phenomena (such as chemistry, deposition, multiple sources, etc.). Within a given flow and dispersion model type, there will be variations in the details on how a specific model handles sources, plume rise, etc. However, many of these details can be modified as needed during the implementation of the models into an operational mode. Thus, the consideration for AOSERP in the selection of a model for subsequent implementation is different than the evaluation of the details of a final version of the model to be used for a particular simulation run.

The USEPA (1978) Workbook referred to in Section 2.2 had 12 application elements, i.e., the equivalent of our "physical processes" (see Table 6). The handling of several of these application elements

Table 6. The application elements in the USEPA (1978) Workbook for comparison of air quality models.

1.	Source-receptor relationship
2.	Emission rate
3.	Composition of emissions
4.	Plume behavior (plume rise)
5.	Horizontal winds
6.	Vertical winds
7.	Horizontal dispersion
8.	Vertical dispersion
9.	Chemistry and reaction mechanisms
10.	Physical removal process
11.	Background, boundary, and initial conditions
12.	Temporal correlations (e.g., correlation between mixing height and stability class)

could be modified readily during the implementation of a model. However, the core of the model (wind and dispersion formulation type) is much more difficult to modify. Thus, the utilization of these application elements was considered to be inappropriate for the objectives of the present study. Rather, the various flow and dispersion types were evaluated in terms of their level of simulation of the winds, mixing processes, and topographic effects, and their adaptability for simulation of source and sink processes.

The physical processes that were utilized in the model evaluation are shown in Table 7. As indicated previously, the flow and dispersion formulations largely determine the levels to which the winds, dispersion, and topography can be simulated. The importance of the level to which these physical processes are simulated will be determined by the specific user needs. These levels have been specified for the first five processes in Table 7. Three of the next physical processes in this table are expressed in terms of the adaptability of the model for their simulation. This was done in order to emphasize that the details of these processes can often be modified during the implemention phase of the models. Although additional parameters such as the mixing height may be very important for the eventual calculation of ground level concentrations, they are usually input data or are calculated outside the flow and dispersion model.

4.3 ASSIGNMENT OF THE APPLICABILITY PARAMETERS

The applicability parameters for each flow and dispersion model type were assigned as a function of each physical process. The value of the parameters ranged from 0 to 10 corresponding to a total inability in simulating the process (0) to a realistic simulation of the process (10). Inevitably, there will be some models of each type which can simulate the processes better or worse than the assigned parameters would indicate. However, it is felt that the applicability parameters should lead to the selection of an appropriate model type.

Table 7. Physical processes and their level of simulation utilized in the evaluation of the flow and dispersion model types.

Physical Process	Level of Simulation
1. Wind Speed:	Uniform Vertical profile Divergence-free profile
2. Wind Direction:	Uniform Vertical profile Divergence-free profile (combined with speed)
3. Topographic Flow:	Horizontal parallel flow Flow changes due to obstacle effect Flow changes due to density-driven flows such as drainage flows
4. Horizontal Mixing:	Uniform in the vertical Height dependent mixing parameters Enhancement due to wind direction shear Terrain-induced changes in mixing parameters
5. Vertical Mixing:	Uniform in the vertical Height dependent mixing parameters Terrain-induced changes in mixing parameters
6. Model Adaptability for Deposition Simulation	
7. Model Adaptability for Air Chemistry and the Dispersion of Multiple Pollutant Species	
8. Model Adaptability for Interfacing a Plume Rise Submodel	
9. Initial and Source-Dominated Stages	
10. Temporal Variations in the Flow and Dispersion Characteristics	

The assigned applicability parameters are shown in Table 8. An explanation for the rationale involved in the assigned parameters is presented in the following paragraphs.

4.3.1 Wind Speed and Flow Model Type

The interpolation wind field type requires some extra effort to ensure that the divergence-free constraint is met. There is also the problem of whether to generate a vertical velocity field or assume it to be zero in the usual case when vertical velocity measurements are unavailable. The availability of an adequate wind field data base upon which to drive the interpolation model is considered under implementation constraints.

4.3.2 Wind Direction and Flow Model Type

A single input flow field can be used to generate a wind direction shear profile. Even though the field is very simple it will be divergence free. The problem will be in the representativeness of the data used to drive the model and in the inability to allow for topographic effects. Interpolation wind fields based on multiple data input locations can be made divergence-free but have the problems outlined above. Potential flow type models usually incorporate a unidirectional flow as a boundary condition and do not simulate direction shear except for topographic effects. The Navier-Stokes types of model similarly do not often include direction effects except in response to topographic effects. The boundary conditions would become considerably more complex.

4.3.3 Topography and Flow Model Type

Interpolation wind fields have the problem of requiring data having sufficient time and space resolution and statistical reliability in order to resolve the topographical effects. The problem is considered to be more than just a data requirement constraint, because the model gives no guidance or feedback as to whether the input data is adequate. In an operational sense, a well-designed data collection system could provide adequate simulation. However, the design and

Table 8. Assigned applicability parameters for flow and dispersion model types as a function of the simulated physical processes.

Physical Processes and Their Levels of Simulation	Flow Model Types[a,b]					Dispersion Model Types[a,b]			
	1	2	3	4	5	1	2	3	4
1. Wind Speed:									
Uniform	10	10	X	X	X	10	10	10	10
Profile (z)	10	10	10	10	10	1	10	1	10
Divergence-free	-	6	10	10	10	-	-	-	-
2. Wind Direction:									
Uniform	10	10	10	10	10	10	10	10	10
Profile (z)	10	10	2	6	6	0	5	0	9
Divergence-free	-	6	2	6	6	-	-	-	-
3. Topographic Flows:									
Horizontal parallel flow	10	10	10	10	10	10	10	10	10
Obstacle effects on flow	0	5	5	7	9	3	7	2	9
Density flows	0	3	0	0	8	0	5	0	7
4. Horizontal Mixing:									
Uniform in vertical	-	-	-	-	-	10	10	0	10
Height dependent	-	-	-	-	-	0	10	0	10
Direction shear effects	-	-	-	-	-	6	5	0	9
Terrain effects	-	-	-	-	-	0	5	0	5
5. Vertical Mixing:									
Uniform in vertical	-	-	-	-	-	10	10	5	10
Height dependent	-	-	-	-	-	0	10	5	10
Terrain effects	-	-	-	-	-	0	5	0	5
6. Deposition Adaptability	-	-	-	-	-	5	8	5	3
7. Air Chemistry and Multiple Species	-	-	-	-	-	2	5	8	2

Continued...

Table 8. Concluded.

Physical Processes and Their Levels of Simulation	Flow Model Types[a,b] 1	2	3	4	5	Dispersion Model Types[a,b] 1	2	3	4
8. Plume Rise Submodel Interfacing	-	-	-	-	-	9	7	5	7
9. Initial and Source-Dominated Stages	-	-	-	-	-	9	5	3	5
10. Temporal Variations	8	8	8	8	8	5	8	8	8

[a]
- = not applicable
x = not applicable because model type is too complex; would need to bypass the more complex model formulation
0,10 applicability parameter range corresponding to inability to simulate (0) to a realistic simulation (10)

[b]Numerical solutions of the advection-diffusion equation

Flow Model Type

1 Single input wind fields
2 interpolation of multiple input wind fields
3 potential flow type wind fields
4 momentum conservation models
5 momentum and energy conservation models

Dispersion Model Types

1 Gaussian dispersion formulations
2 Eulerian
3 Lagrangian
4 Particle-in-cell

operation of such a system would be difficult to adequately achieve without the utilization of more advanced modelling techniques.

The potential flow types of models cannot simulate flow separation. In addition, this model type requires careful calibration of model parameters to simulate the effects of stability. Nevertheless, the gross features of the flow can be estimated, particularly with the more advanced models in this class.

The momentum equation (Navier-Stokes) models can simulate flow separation. However, calibration of model parameters for stability effects is required.

The momentum plus energy class of models can generally simulate the atmospheric stability effects upon the flow parameters; however, computer restraints may present problems in obtaining resolution. In addition, the simulation may suffer from inadequate boundary condition specification. The drainage flows, in particular, may require very detailed specification of the lower boundary conditions and their variations which are very difficult to attain in operational or even in most field validation conditions.

4.3.4 Wind Speed and Dispersion Types

The Gaussian formulation can adopt the mean wind speed of the centreline height; otherwise a wind profile cannot be simulated. Lagrangian models usually are of the moving box type in which vertical variation of the wind speed and direction is ignored. However, an optimum wind speed based upon the assumed height of the centre-of-mass of the pollutant can be incorporated.

4.3.5 Wind Direction and Dispersion Types

Eulerian grid models often have serious numerical dispersion problems associated with finite differencing of the advection term in the advection-diffusion equation if the flow is significantly non-unidirectional. A variety of techniques have been developed to attempt to overcome this problem (see Section 3); however, many models of this type simply assume a unidirectional wind field. The particle-in-cell type models can handle the wind direction shears; however, the set-up of the dispersion model may be more complex.

4.3.6 Topographic Flows and Dispersion Types

Gaussian models can be applied around a centreline defined by a streamline generated by a flow model. However, the convergence of the flow is not simulated in a Gaussian formulation. In a usual Gaussian formulation, the flow model is very primitive involving only rudimentary allowance for terrain. Lagrangian models could have trajectories modified by terrain if linked to the appropriate flow model. However, vertical variations in ground level are often neglected.

The Eulerian dispersion models may have numerical dispersion problems associated with the non-uniform wind direction in terrain-modified flow fields. The density flows in particular may have the additional complexity of distinctive mixing parameters within the space-limited density flows which cannot be well specified. The particle-in-cell dispersion formulations have the similar problem of diffusion coefficient specification.

4.3.7 Horizontal Mixing and Dispersion Types

The resolution of the effects of wind direction shear upon lateral dispersion requires the proper simulation of both the wind direction shear and the vertical mixing, both of which may be highly dependent on stability variations. In a Gaussian formulation, the contribution to lateral dispersion from shear effects can be calculated externally to the model and then the modified σ_y values can be applied. Although linear wind shear effects upon the lateral dispersion can be fairly readily accounted for analytically, externally to a Gaussian formulation (see Pasquill 1974; Davison and Leavitt 1979), most applications of Gaussian models have adopted standard sigma curves and the shear effects have been ignored. Shear dispersion effects will increase the dispersion effects and, for the "worst case" situation, their neglect is of no particular concern.

The direction shear effects would be automatically simulated within a k-theory dispersion framework if wind direction shear effects are included in the flow field. However, the numerical dispersion problem discussed previously applies. The terrain effect of increasing the amount of mixing due to enhanced mechanical energy production can be approximated in k-theory Eulerian or particle-in-cell models by linking the diffusion coefficient to changes in the velocity field. Complications include the calibration of the enhanced coefficients, including stability effects, and the specification of turbulent wakes beyond the region of increased flow.

4.3.8 Vertical Mixing and Dispersion Types

The same comments apply to vertical mixing as to horizontal mixing except that some Lagrangian models have an explicit vertical diffusion formulation.

4.3.9 Deposition, Adaptability, and Dispersion Types

Deposition probably does not need to be coupled to the dispersion formulations within perhaps 50 km of the source (see Section 2). Thus, if necessary, deposition can be estimated from the ground level concentrations by adoption of a suitable deposition submodel external to the dispersion model calculations.

In the Gaussian dispersion formulation, deposition can be coupled to the dispersion formulation by modifying the source strength of the virtual image sources. However, spatial variations in the deposition cannot be readily accounted for.

In the Eulerian k-theory dispersion models, deposition can be explicitly accounted for; spatial variations could also be included. In a particle-in-cell model, a decision algorithm would have to be included to determine if a particular particle is absorbed or reflected; this may introduce some difficulties, especially considering the integral nature of the particles. The Lagrangian k-theories can allow for deposition but often instantaneous vertical adjustment of concentration may be assumed.

4.3.10 Air Chemistry, Multiple Species, and Dispersion Types

Air chemistry is probably best handled by vertically integrated Lagrangian type models or else simple box models. Simple linear chemistry can be handled by Eulerian models by adoption of bulk reaction rates or using a half-life approach. However, multiple species and complex chemical reactions are seldom explicitly included in a three-dimensional Eulerian grid model. Gaussian models can be formulated to allow for changing source strength as a function of downwind distance in order to simulate the effects of chemical reactions with a known effect. The integral nature of the particles in a particle-in-cell approach means that simulation of a non-passive contaminant is difficult except by allowing a decreasing amount of pollutant to be represented by each particle.

4.3.11 Plume Rise Submodel Interfacing and Dispersion Types

Plume rise can be calculated either totally externally to the flow and dispersion model or else as a submodel. The plume rise often is incorporated by means of a virtual source at a height given by the effective stack height. However, plume rise may continue for some distance downwind, particularly in neutral conditions (Briggs 1975) and an effective stack height is not totally adequate. A Gaussian model probably can be more readily modified to allow for continued plume rise than Eulerian or particle-in-cell type models because each source is kept separate. Lagrangian models often are vertically integrated so that plume rise is not considered at all. Even if a Lagrangian model does have vertical diffusion, the sources are not kept separate.

4.3.12 Initial and Source-Dominated Stages and Dispersion Types

The initial stage of dispersion is known to be source-dominated (see for example Briggs 1975, Davison and Leavitt 1979). Thus, models based on environmental mixing, may incorrectly simulate dispersion close to the source. For elevated plumes on flat terrain, the plume effluent will not impinge upon the ground until the environmentally dominated dispersion stage is well established (Pasquill 1976). It is also well known that k-theory has limitations until dispersion times of perhaps two or more Lagrangian integral time scales (see discussion in Section 3). Thus, the application of environmentally determined k-values, close to the source, may be inappropriate. For many practical applications, however, these limitations may not be important. In a Gaussian dispersion model, these initial effects can be readily accounted for by adopting the appropriate sigma values.

4.3.13 Temporal Variations of Flow and Dispersion Characteristics

Most models have some ability to account for changed conditions. However, for flow fields, a typical procedure is to calculate a series of steady state conditions. Often, there are no better data to drive the models. For the dispersion model types, the numerical solutions of the advection-diffusion equation are often formulated to permit modification of the dispersion coefficients maintaining a "restart file" of the previous concentrations. If not, a series of steady state solutions must be utilized as an approximation. Gaussian models are generally forced to use this latter procedure. Even time-dependent puff models of the Gaussian type seldom permit variations of the dispersion parameters.

5. IMPLEMENTATION CONSIDERATIONS FOR MODEL TYPES

5.1 SELECTION OF IMPLEMENTATION CONSIDERATIONS

The problems and cost involved in implementing an air quality simulation model are often a major concern. The importance of implementation considerations depends to some extent upon the user. For this reason, many model reviews have not attempted to include them (e.g., USEPA 1978; IEC 1975). However, it is still possible to evaluate model types reasonably objectively in terms of the relative complexities of the implementations. A series of relative implementation parameters can serve as an aid in the eventual model selection.

Implementation considerations can be grouped into three areas of major concern. These are:

1. The input data needed to drive the models;
2. The computer requirements; and
3. The technical level of personnel required to set up and run the models.

All three of these areas impact upon the eventual cost and feasibility of implementing a particular air quality model by an individual user.

Implementation parameters can be assigned to various levels within each of these three areas of concern depending upon the difficulty and/or cost of the particular level. The assigned implementation parameters are shown in Table 9. Although they are rather arbitrary, the implementation parameters do reflect the gradations involved in the implementation considerations. Whether or not the area of concern is important becomes a function of the specific program of the individual user.

5.2 THE ASSIGNMENT OF IMPLEMENTATION PARAMETERS TO MODEL TYPES

Implementation parameters were assigned to the various flow and dispersion model types as functions of the stage of model implementation and the complexity of the environmental situation being simulated. These implementation parameters are shown in Table 10; the

Table 9. Implementation parameters defined by the levels of complexity for the various areas of concern in the implementation process.

Areas of Concern for Implementation	Levels of Complexity	Implementation Parameter
Input data requirements	- routinely available or data not needed	10
	- additional processing of routine data	9
	- collection of more data with a routine system (e.g., higher density of measurements)	<7
	- collection of more data with a complex system	<5
	- very difficult to attain adequate input data	0
Computer requirements	- analytic solution, no computer	10
	- minicomputer for a short time	8
	- minicomputer for a long time	5
	- large computer for a short time	5
	- large computer for a long time	2
Technical personnel requirements	- routine operation, technician	10
	- some dispersion meteorological experience required, involving a meteorologist/engineer	6
	- experienced dispersion meteorologist/modeller	2

Table 10. Implementation parameters for model types. The meaning of the values of the parameters was outlined in Table 9.

Physical Processes and Their Levels of Simulation	Flow Model Types[a,b] 1	2	3	4	5	Dispersion Model Types[a,b] 1	2	3	4
1. Input Data for Model Calibration and Site-Specific Tuning:									
No topography, simple meteorology	N	7	7	7	7	6*	5	5	5
Complex topography	N	4	6	6	6	4*	4	4	4
Complex meteorology	N	5	7	7	7	N	5	5	5
Complex energy boundary conditions	N	N	N	N	3	N	3	3	3
2. Input Data for Operational Use:									
No topography, simple meteorology	10	10	10	10	10	9*	9	9	9
Complex topography	N	6	9	8	8	9*	9	9	9
Complex meteorology	N	7	9	8	8	N	9	9	9
Complex energy boundary conditions	N	N	N	N	5	N	4	4	4
3. Computer Requirements:									
Normal operations	10	7	5	3	2	8	4	6	2
4. Technical Personnel Requirements:									
Initial set-up and site-specific tuning	N	2	4	2	2	6	4	4	4
Routine operations	6	4	4	2	2	6	4	4	4

[a]N = not applicable
* = The application of Gaussian formulations in complex terrain has major technical limitations.

[b]Numerical solutions of the advection-diffusion equation

Flow Model Type		Dispersion Model Types	
1	single input wind fields	1	Gaussian dispersion formulations
2	interpolation of multiple input wind fields	2	Eulerian
3	potential flow type wind fields	3	Lagrangian
4	momentum conservation models	4	Particle-in-cell
5	momentum and energy conservation models		

rationale for the assigned values is discussed in the following paragraphs.

5.2.1 Input Data for Model Tuning

The initial site-specific model tuning of the flow field requires assurance that the parameters used to drive the flow field are appropriate. Even in seemingly simple situations, the correctness of the assumed simplicity should be verified by actual measurements. In complex terrain, the adequacy of the system of data sites for interpolation of the wind field should be verified. More complex models should be capable of generating the major features of the flow field with standard parameters and measurements are needed only to fine tune the model parameters. Unlike the interpolation flow model types, the more complex model types would give good guidance as to how to proceed with the validation and site-specific tuning. The same types of considerations apply to complex meteorological situations. For momentum and energy conservation flow models, the spatial variations of the lower boundary condition may require an extensive data base in order to properly specify it.

The type of data required to fine tune the dispersion models is not too sensitive to the type of formulation employed. In all cases, the data collected consist of pollutant concentrations as field variables together with the associated meteorological conditions. The data are generally more difficult to determine reliably in complex topography or during complex meteorological conditions. The data for the more complex models may have to be processed in a more complex manner; this difference is also reflected in the technical personnel requirements discussed below.

5.2.2 Input Data for Operational Use

When the models have been tuned to the particular site, then only routinely available data should be required for the simple meteorological situations. In more complex meteorological situations and in complex terrain, the models incorporating calculated wind fields should require only the boundary conditions to generate reasonable flow fields. However, models with an interpolation wind field will still require significant data input, even through the tuning of the model would ensure that this operational requirement is optimized.

The dispersion simulations for tuned models similarly should require only limited data to operationally run the models after site-specific tuning is completed.

5.2.3 Computer Requirements

Computer requirements are probably the most difficult of the implementation considerations to generalize. There is much variation between specific models of the same model type depending upon the solution formulation and technique. The resolution and complexity of the particular application also have a major influence on the computer requirements and runtime. The assigned implementation parameters in Table 10 give some indication of the relative computer requirements; however, the costs probably do not scale with the inverse of the parameter value.

Although computer size requirements are often rated as fairly important by many users, the advent of convenient, remote, time-share computer systems means that powerful machines are accessible for quite modest costs to small users. Thus, the present authors are convinced that the level of technology required to meet user needs should have predominance over the desire to design the model for operation on smaller computers.

5.2.4 Technical Personnel Requirements

The complexity of the particular application determines the level of technical personnel required for the initial model set-up and site-specific tuning. If there is no significant topography and if simulations in relatively straightforward meteorological situations are desired, then the model tuning is minimal and standard procedures can be followed. In areas of complex terrain or in complex meteorological situations, an experienced dispersion meteorologist or equivalent is clearly required for model tuning.

It should be emphasized that air quality models are tools and that the results obtained from the application of any tool are a function of both the quality of the tool and the experience of the craftsman. There has been an unfortunate trend in air quality studies for organizations to assign new personnel with relatively little experience in air quality meteorology to undertake dispersion calculations using available models. The results are sometimes dismal and the blame may be placed on the tool rather than on the inexperience of the person setting up and running the model.

Therefore, even in routine operations, a trained air quality meteorologist/engineer is required to adequately run the models. In applications such as use of the momentum-conservation flow models in complex terrain and in complex meteorological situations where modelling technologies are being pushed to their limits, a dispersion meteorologist is required to ensure proper application of the model and recognition of the limits of the reliability of the results.

6. RECOMMENDED MODEL TYPES FOR IDENTIFIED USER NEEDS

6.1 PROCEDURE FOR MODEL SELECTION

In the preceding sections, user needs have been identified and described in terms of required model characteristics. Model types have been described and their abilities to describe various physical processes have been quantified in terms of application parameters. The difficulties of implementation of model types have been quantified in terms of implementation parameters. In this section, the identified user needs are reviewed in terms of how well the various physical processes need to be simulated. In this way, importance parameters corresponding to the application parameters can be generated for each identified user need. A large value of the importance parameter means that that level of simulation of the physical process is important for the particular user need. A low value of the importance parameter means that that level of simulation is inadequate. An initial technical selection of models can then be performed based on the products of application and importance parameters. Implementation parameters are then considered for each user need to generate recommended models.

In practice, a strictly objective weighting of model types was not possible. The application parameters presented earlier reflect the limitations of the model types in a wide variety of applications. For a given user application, some of these model limitations are of no concern and a re-assessment of the parameters for each particular user need was required. The adopted methodology involving parameters did, however, ensure that all advantages and disadvantages of model types were systematically considered; even though a simple summation of products of the parameters was not considered appropriate.

In the following sections, recommended model types were selected for the identified user needs discussed in Section 2 (see Table 3). The short-term, real-time predictive models for supplementary control systems and the long-range trajectory transport problems were considered to be user needs not pertinent to AOSERP directly; thus, only the second, third, and fourth types of user needs in Table 3 are considered below. Since several model types will be recommended, from a consideration of the distinct user needs, a synthesis of the recommended model types recognizing the overlap in model requirements is made in Section 6.6.2.

6.2 WORST CASE SIMULATIONS FOR REGULATORY STANDARDS

6.2.1 Assignment of Importance Weighting Parameters

The first identified user need of direct concern to AOSERP is the need for models to aid in the maintenance of regulatory air quality standards. As discussed in Section 2.3.2, the requirement here is for the accurate simulation of worst case situations. These worst case simulations do not need to be governed by measured meteorological data; rather, the meteorological parameters (mixing height, wind speed, stability, etc.) can be varied to determine the worst case situation.

The importance weighting parameters for each of the physical processes outlined in Table 7 are assigned in Table 11. A high value of the parameter implies that that level of simulation of the physical process is important for the user need; a low value mean that that level of simulation is inadequate. The rationale for the parameter values is discussed in the following paragraphs.

6.2.1.1 Wind speed parameters. In flat terrain and with site-calibrated dispersion coefficients, it does not appear to be necessary to simulate a realistic wind profile for worst case simulation. Although a wind profile obviously exists, a calibrated model probably does not need to explicitly simulate it in order to achieve sufficiently accurate concentration estimates.

In complex terrain situations, however, realistic terrain-effect simulations will probably require a divergence-free wind field.

Table 11. Importance weighting parameters for various physical processes for each of the identified user needs.

Physical Processes and Their Levels of Simulation	Classes of User Needs[a]			
	Regulatory Standards		Frequency Distribution	
	T	NT	T	NT
1. Wind Speed:				
Uniform	2	10	2	10
Profile (z)	2	10	2	10
Divergence-free	10	10	10	10
2. Wind Direction:				
Uniform	10	10	8	8
Profile (z)	10	10	10	10
Divergence-free	10	10	10	10
3. Topographic Flows:				
Horizontal parallel flow	2	10	2	10
Obstacle effects on flow	10	N	8	N
Density flows	-	-	10	-
4. Horizontal Mixing:				
Uniform in vertical	4	10	3	6
Height dependent	4	10	4	8
Direction shear effects	-	-	5	10
Terrain effects	8	N	8	N
5. Vertical Mixing:				
Uniform in vertical	4	10	4	10
Height dependent	4	10	5	10
Terrain effects	8	N	8	N
6. Deposition Adaptability	-	-	5	5
7. Air Chemistry and Multiple Species	-	-	-	-

Continued...

Table 11. Concluded.

Physical Processes and Their Levels of Simulation	Classes of User Needs[a]			
	Regulatory Standards		Frequency Distribution	
	T	NT	T	NT
8. Plume Rise Submodel Interfacing	10	10	10	10
9. Initial and Source-Dominated Stages	5	-	5	-
10. Temporal Variations	-	-	-	-

[a]T = Terrain
NT = no terrain
N = not applicable
\- = unimportant

0,10 importance weighting parameters, corresponding to a level of simulation that is important to achieve for the particular user need (10), to an inadequate level of simulation (0).

6.2.1.2 Wind direction parameters. Since worst case simulations are desired, a uniform wind direction appears to be adequate. Shear-enhanced dispersion would generally not be important at the downwind distances of concern for maximum concentrations and it represents an occasional additional dispersive mechanism which can be ignored for worst case simulations.

6.2.1.3 Topographic flow parameters. In flat terrain situations, horizontal parallel flow is adequate. In complex terrain situations, simulation of the obstacle effect upon the flows is highly desirable. The adoption of terrain-following flow or half-terrain models does make some allowance for topography; the flow formulation is essentially the same as for horizontal parallel flow. Because the authors feel that this type of response to topographic effects is not very adequate, an important weighting parameter of 2 has been assigned.

6.2.1.4 Horizontal mixing parameters. In flat terrain, the adoption of site-calibrated dispersion parameters should probably lead to adequate horizontal mixing simulations for worst case situations. In complex terrain, the terrain can be expected to enhance the dispersion. The site-specific calibration of these effects may be difficult to achieve. Since terrain and roughness effects are known to result in significant changes in dispersive characteristics (see for example Islitzer and Slade 1968:133 ff.), the inclusion of these effects is important for accurate predictions.

Direction shear effects will not be of importance for worst case simulations.

6.2.1.5 Vertical mixing parameters. The same comments apply to vertical mixing as were outlined above for horizontal mixing.

6.2.1.6 Deposition and air chemistry parameters. Sink mechanisms are of little concern for worst case simulations for regulatory standards.

6.2.1.7 Plume rise parameters. For worst case simulations, the adoption of an effective stack height is probably an adequate formulation. The question of whether plume rise continues in neutral conditions beyond the point of maximum ground level concentrations is of little concern for a worst case simulation. The adoption of a correct plume rise is vital to accurate predictions; however, it is felt that sufficient work has been done on plume rise to ensure that an adequate estimate can be made external to the dispersion model.

6.2.1.8 Initial and source-dominated stage parameters. As discussed in Section 4, the plume generally will not give significant ground level concentrations in flat terrain until the initial effects are negligible. In a complex terrain situation where the terrain rises significantly within 2 or 3 km of the source, then initial and source-dominated effects may be important.

6.2.1.9 Temporal variation parameters. For worst case simulations, the adoption of a steady state condition should be adequate.

6.2.2 Selection of Model Types for Flat Terrain--Regulatory Standards.

The importance parameters of Table 11 under the heading "Standards, NT" combined with the applicability parameters of Table 8 show that there are no significant technical preferences for the flow type. For no topography and simple meteorology, the implementation parameters of Table 10 give a preference for a single input flow field (type 1). However, all other flow types could also be adopted if a more powerful model is required for another application.

The applicability parameters for the dispersion model types indicate that the Lagrangian formulation (type 3) is inadequate due to poor mixing formulations. The Gaussian formulation has an advantage in plume rise formulations as shown by the applicability parameters; however, for the standards application, continued plume rise is of no concern and the differences in the applicability parameters between dispersion types 1, 2, and 4 are irrelevant. Thus, from a technical viewpoint, only dispersion type 3 is inadequate; other forms are all equally acceptable.

For the standards application, site-specific tuning of the dispersion parameters is important. The tuning of more complex models may require more data analysis by more highly trained personnel. The advantages of reduced computer requirements and reduced technical personnel requirements mean that a Gaussian dispersion formulation is optimum for this application.

In summary, for the maintenance of regulatory standards in flat terrain situations, the use of a Gaussian dispersion formulation and a simple flow field specification is adequate. Other model types could work as well technically; however, there are implementation disadvantages. Site-calibrated dispersion parameters are required for acceptable accuracies.

6.2.3 Selection of Model Types for Complex Terrain--Regulatory Standards

The complexity of the topography largely determines the technical requirements for the model type. If flow separation is important, then flow types 4 and 5 are adequate with flow type 2 (interpolation wind fields) being less accurate. The input data requirements for an interpolation wind field approach (lower implementation parameters in Table 10) are considered to be a major disadvantage to this approach. For studies involving regulatory standards, it may be optimum to use a more limited data set to tune the more complex models which can then be used to generate the "worst case" situation.

If flow separation is not important for the regulatory standards application, then flow type 3 (potential flow type model) is technically adequate and has implementation advantages over flow type 2 (interpolation wind field) in the input data required to tune and run the model. Flow types 4 and 5 have implementation disadvantages (computer and personnel) compared to flow type 3.

The dispersion formulations for the standards application in complex terrain need to be considered carefully. The wind speed and and direction formulations are not major determinants for the dispersion type. The topographic flow applicability parameters reflect the weakness of the Gaussian model in terrain flow conditions. Dispersion type 3 is inadequate due to poor horizontal mixing simulation. The advantages of the Gaussian model for continued plume rise are considered unimportant for a standards application. For the initial effects consideration, a Gaussian formulation has an advantage. If there is significant rising terrain (up to effective stack height) within a couple of kilometres of the source, then a Gaussian dispersion formulation could perhaps be coupled onto a k-theory for the first kilometre to allow for initial effects prior to terrain effects becoming important. If the terrain obstacles are farther downwind, then the importance of initial effects is much less. Alternatively, modified dispersion coefficients following the predictions of Taylor's statistical theory and source-dominated dispersion theory could also be used closer to the source.

The implementation considerations for the complex terrain situation give the Gaussian approach (dispersion type 1) an advantage in the technical personnel and computer requirements compared to flow type 2 (Eulerian k-theory). However, it is felt that the implementation advantages are not so great as to offset the serious technical deficiencies of the model. Dispersion type 4 (particle-in-cell) has the disadvantage of having significantly larger computer running costs. The technical advantage of dispersion type 4 in reducing numerical dispersion effects may not be too important since uniform wind directions are considered adequate for a worst case simulation in the AOSERP terrain situations.

In summary, for moderate terrain (no flow separations), a potential flow type of model combined with an Eulerian k-theory is optimum. For severe terrain (flow separations), the flow field simulation would require a momentum and energy conservation model type.

An interpolation wind field could be used in both situations; however, it has some technical and more serious implementation disadvantages.

6.3 FREQUENCY DISTRIBUTIONS WITH STRATIFICATION PARAMETERS

6.3.1 Assignment of Importance Weighting Parameters

Another major identified user need is the need for models which can provide frequency distributions of ground level (i.e., canopy top) concentrations with appropriate stratification parameters. As discussed in Section 2.3.2, the stratification parameters could include solar insolation, temperature, surface moisture, etc. A variety of specific applications are envisaged and the selection of the stratification parameters should be flexible and be a run-time variable if possible. Hourly predictions over selected seasons or times are probably most useful. These series of steady-state solutions could then be combined to generate frequency distributions or other statistics as desired. An important characteristic of this application is that many separate simulations or realizations are averaged. Thus, a larger error in the accuracy of each prediction is acceptable as long as the error is not systematic.

The importance weighting parameters are shown in Table 11. The rationale for the parameter values is discussed in the following paragraphs. As for the standards application discussed above, terrain and non-terrain situations have been separated.

6.3.1.1 Wind speed parameters. For flat terrain and with site-calibrated dispersion parameters, it does not appear to be necessary to simulate a realistic wind profile. The averaging of many realizations means that the variance introduced by such an approximation is not important in the flat terrain situation. In complex terrain, however, a realistic flow field is required since large systematic errors could otherwise result.

6.3.1.2 Wind direction parameters. For the development of frequency distributions, we need to deal with real data. Thus, the location of ground level concentrations may be affected by a wind direction profile. Clearly the wind direction data used to determine the trajectory of the plume must be the wind direction near the height of the plume centreline. However, the area on the ground exposed to the concentrations may be different due to a wind direction profile. In most applications of this type, wind sector-averaging is used. This means that all winds from a particular solid angle are lumped together for the frequency distribution. Thus, in practice, the need for resolving the wind direction profile is not too important.

6.3.1.3 Topographic flow parameters. In flat terrain, horizontal parallel flow is adequate. In complex terrain, the flow modifications due to the terrain will cause major systematic differences to the ground level concentrations. Wind angle sector-averaging and averaging over many realizations does not remove this difficulty. The adoption of terrain-following flow or half-terrain models is not very instructive, particularly in a three-dimensional terrain situation. These types of flow formulations have been classified in Table 11 as horizontal parallel flow.

6.3.1.4 Horizontal mixing parameters. In flat terrain, site-calibrated dispersion parameters are generally adequate. Shear-enhanced dispersion may be important at downwind distances greater than about 10 km. The occurence of shear-enhanced dispersion is not too common; even for the longer distances. The effect is not critical due to the averaging over many realizations; only some of which are affected by shear-enhanced dispersion. The real atmosphere will have variations of mixing with height. The adoption of a single mixing or stability class is a very rough approximation. However, the process of averaging over many realizations means that the averaged output may not be seriously in error.

In complex terrain, the above considerations all apply; however, there is the additional effect of terrain-enhanced mixing. The terrain-enhanced mixing can be reasonably compensated in moderate rolling terrain by site-specific diffusion coefficients which are spatially invariant. In major terrain, the specific terrain-induced effects are more important and spatially varying diffusion coefficients generated from the flow field are desirable.

6.3.1.5 Vertical mixing parameters. The relative magnitude of parameters is similar to those for horizontal mixing. Terrain enhancement is systematic and should be included.

6.3.1.6 Deposition parameters. An average deposition is desirable for the frequency distribution models. As mentioned in Section 2.2.1, deposition can probably be decoupled from the dispersion model for the first 50 km or so. However, it would be convenient to provide first-order estimates of the deposition in a frequency distribution model. The deposition rate should be a function of the stratification parameters.

6.3.1.7 Plume rise parameters. The formulation of plume rise and its relation to the mixed layer height is important on a case-by-case simulation. The averaging over many realizations, however, permits the adoption of a simplified model which may result in an increased variance of the predicted to observed ratios for concentrations as long as the population average is not seriously affected. For this reason, a detailed boundary layer description interfaced with the plume rise is probably not required. Reasonably accurate plume rises and boundary layer heights, however, must be available for accurate, averaged simulations.

6.3.1.8 Initial and source-dominated stage parameters. As for the standards application discussed in Section 6.2.1, the initial effects may be important where rising terrain occurs within 2 or 3 km of the source.

6.3.2 Selection of Model Types for Flat Terrain--Frequency Distributions

The application parameters for the flow types gives a slight preference to input and interpolation wind fields due to the wind direction consideration. However, as discussed above, the sector averaging over many realizations means that this advantage is not significant. Implementation considerations give a clear advantage to the simple input flow field. In complex meteorological situations, flow types 2 or 3 (interpolation or potential flow) are desirable. However, averaging over many realizations probably means that accurate simulation of complex meteorology is unnecessary.

For the dispersion formulation, the Gaussian formulation has a technical limitation in having uniform mixing in the vertical. Dispersion types 2 and 4 (k-theory and particle-in-cell) have advantages over the Gaussian in mixing simulations. Dispersion type 3 (Lagrangian) has no lateral mixing and is considered technically inadequate.

Deposition was assigned an importance rating of 5 in Table 11. Gaussian formulations were assigned an applicability factor of 5 having the drawback of lack of spatial variations. Particle-in-cell formulations (applicability parameter of 3) are not well suited for deposition. The Eulerian k-theory formulations can easily include a spatially varying deposition formulation. However, it is reasonable to decouple the deposition from the dispersion calculations and calculate deposition estimates from the ground level concentration patterns. Thus, there is only a slight advantage for the Eulerian simulations.

The application considerations of the dispersion formulations lead to a mixed technical evaluation. The Gaussian technique (type 1) has some limitations in the deposition formulation; however, a decoupled deposition submodel could be linked fairly easily to it. The Gaussian formulation has the additional disadvantage of assuming uniform mixing. This limitation introduces a larger variance in the prediction errors; however, the averaging over many realizations for the frequency distribution application lessens the significance of this limitation. The Gaussian formulation can include shear-enhanced dispersion if the sigma coefficients are properly formulated; however, the frequency of occurrence and the availability of routine input data to specify it may not be sufficient to warrant special allowance for this effect. The Eulerian k-theory (type 2) models have a disadvantage in usually having numerical dispersion problems if shear-enhanced dispersion and a wind direction profile are included. This limitation is probably not important for the reasons discussed above. The particle-in-cell dispersion type (type 4) is technically good except that deposition is hard to handle; a separate deposition submodel would be required.

Implementation consideration from Table 10 gives a clear advantage for the Gaussian formulation with the particle-in-cell approach being particularly poor due to computer requirements. Of special consideration for the application of calculating stratified frequency distributions is that the data required to drive the models on a climatological basis may not be very extensive, especially in terms of vertical profiles.

In summary, a Gaussian dispersion model with a single input wind field is adequate. Only if complex meteorology is of concern and if sufficient data are available do a more complex dispersion formulation (type 2) and flow formulation have an advantage.

6.3.3 Selection of Model Types for Complex Terrain--Frequency Distributions

The application parameters for flow model types in complex terrain situations give a clear advantage to the more complex flow types compared to the single input flow field. From implementation considerations, flow type 3 (potential flow type) has advantages over flow type 2 (interpolation type) and the more complex formulations 4 and 5. In evaluating the implementation considerations, a higher importance was assigned to the disadvantage of continued data requirements and the associated uncertainties inherent with flow type 2 compared to the increased computer requirements of flow type 3.

There may be situations in which flow separation is an important feature. The routine running of the more complex flow models 4 and 5 could become very expensive. In such situations, the identification of a limited number of flow classes would permit a very limited running of the complex flow models for, perhaps, only a limited set of wind directions. For wind directions where flow separation is not a problem, simpler flow-types could be used. Similar considerations could apply if drainage effects are very significant; in that case, flow model type 5 (momentum and energy) might be required.

The dispersion technical considerations include the additional effects of the topographic flows and the enhanced mixing compared to the flat terrain case. The distortion of the flow field means that the Gaussian formulation requiring uniform mixing and dispersion has serious technical drawbacks. Dispersion type 3 (Lagrangian formulation) is probably inadequate due to the lack of horizontal mixing. The effects of shear-enhanced dispersion are considered to be of minor importance for inclusion in a model for a frequency distribution application due to the limited occurrence of the effect and the probable difficulty of obtaining climatological data to reasonably estimate the effect. It is recognized, however, that for some stratification parameters, the neglect of shear-enhanced dispersion could result in the prediction of higher concentrations over more spatially limited areas than would actually occur. Note that the ground level concentrations averaged over many events probably would not be significantly affected due to the averaging implicit in this particular model application.

The implementation considerations are similar to those for the standards application in complex terrain. Interpolation models required substantial input data and technical expertise to set them up. Subsequently, they continue to require substantial input data to run. Particle-in-cell models are generally considered expensive to run and do not appear to provide a compensating technical advantage for this user need.

In summary, if there is significant terrain, then a potential flow type of model with an Eulerian k-theory dispersion formulation is optimum. In severe terrain, with flow separations, a momentum or momentum plus energy flow model may be required. For a frequency distribution application, a complete wind direction frequency is usually run. Often only a few directions are subject to major terrain influences. Then, a combination of models might be run with the more complex (and costly) models (particularly flow types 4 and 5) being limited to only a few wind directions. Flow type 3 (potential flow type) is often not too expensive to run and the additional work associated with trying to combine it with a Gaussian in some directions may not be worthwhile.

6.4 LONG-TERM DEPOSITIONS

6.4.1 Similarity to Model Requirements for the Frequency Distributions Application

For long-term depositions, individual realizations become less and less important. Any model that satisfies the frequency distribution requirement will be adequate for the deposition requirement, although a separate deposition submodel may be required if the model does not handle deposition well. If models to satisfy the frequency distribution application are to be run, then the long-term deposition application can be satisfied by suitable manipulation of the available output, since migration of deposited material within the soil is generally considered to be slow. Terrain effects are still not negligible since large systematic discrepancies may be expected. An exception to this conclusion may be an acid flush in the spring which may remove much of the deposited material in the snow if it is soluble. However, this process can be allowed for by keeping a seasonal frequency distribution in the long-term deposition.

6.5 LONG-RANGE TRANSPORT

Although long-range transport may not have a high priority at this time for AOSERP, it is recognized that interprovincial transport of pollutants may become an important user need in the future if several plants are constructed in the oil sands region. The additional technical consideration for long-range transport models is that a time-varying trajectory will be required. The initial plume rise and dispersion problems become very much less important as do individual realizations. At the present time, AES is developing long-range transport models. If long-range transport becomes a major concern for AOSERP, then the AES models should provide a useful basis upon which to build.

6.6 SYNTHESIS OF RECOMMENDED MODEL TYPES

6.6.1 Summary of Recommended Models

The analyses in the previous sections led to the recommendations of several model types. In flat terrain, a single input wind field and a Gaussian dispersion formulation are considered adequate for both standard and frequency distribution applications. In moderately complex terrain, a potential flow model (with a reasonable allowance for the surface boundary layer through either a coupled boundary flow model or a modified potential flow concept) is recommended along with a k-theory dispersion formulation. In severe terrain situations with flow separations or for drainage flow situations, a momentum and energy conservation flow model is recommended.

6.6.2 Comments on the Rationale for the Recommended Models

The identified user needs played a major role in the selection of the recommended models. For the application involving the maintenance of regulatory standards, worst case hypothetical situations, not real data, could be used to describe the meteorology. For the frequency distribution application, the averaging over many realizations was permitted. The very significant result of these two different characteristics was that real physical processes, such as the evolution of the boundary layer, the vertical profile of the wind direction, and shear-enhanced dispersion, became much less important. The relaxation of the requirement for hour-by-hour accuracy (the type of accuracy of more importance for a supplementary control system for instance) meant that the physical situations being simulated could be simplified, so that the numerical dispersion problems common in the the Eulerian k-theory formulations were not critical. If a directional wind profile is desired or if the terrain-induced flow is significantly non unidirectional for an appreciable distance, then k-theory still could be used if an appropriate numerical technique or sufficiently dense grid spacings are utilized.

The recommendation for Gaussian models in flat terrain situations may be met with some disapproval by process-oriented modellers. However, the authors feel that, for the identified user needs for AOSERP, a Gaussian model in flat terrain is adequate if site-specific dispersion coefficients are employed. The question of whether the terrain in the AOSERP region is "flat" is discussed in Section 7.

The interpolation wind model type was rated generally as fair in the application considerations for complex terrain. However, it was felt that the input data requirements to obtain a reasonable flow field definition were onerous. The measurement provided by a single pibal release has serious statistical sampling problems. Without guidance by a numerical model and without expert analysis of sampling and siting problems, the attainment of even reasonably accurate interpolation wind fields (in order to achieve the "fair" technical rating) is very difficult.

The particle-in-cell dispersion model type had a major drawback of large computer costs. Although the technique is an elegant way of overcoming numerical dispersion problems, the reduced requirement for such advantages due to the user needs analysis meant that the implementation disadvantages were always rated as more important. A developmental program involving the interfacing of the particle-in-cell dispersion model to a potential flow type wind field incorporating a wind direction profile could be worthwhile if the problem of the large computer costs could be overcome.

7. RECOMMENDED MODEL IMPLEMENTATION PROCEDURES

Section 6 analyzed the model requirements to satisfy the identified user needs. In the following paragraphs, specific recommendations are made to synthesize and analyze the AOSERP data bank and to implement specific models. The recommendations are based upon the analysis presented in Section 6.

7.1 GAUSSIAN FREQUENCY DISTRIBUTION MODELS

The flat terrain assumption is probably reasonable as a first approximation for the region affected by the major existing sources, and so a site-tuned Gaussian type model should be implemented. A version of the EPA CRSTER model could be used as a starting point. The model should be modified to permit greater flexibility in the selection of run-time stratification parameters (such as surface moisture, season, time of day, etc.) and to incorporate greatly enhanced statistical output routines. The Pasquill-Gifford-Turner dispersion scheme should be a modified to recognize the serious stability class selection problem identified by Davison and Leavitt (1979); a modified sigma specification scheme based upon AOSERP data is highly recommended.

The processing of the routine climatological data base to be suitable for run-time stratification parameter selections is recognized as a major task.

7.2 SITE-TUNED GAUSSIAN MODELS FOR REGULATORY STANDARDS

Assuming that the flat terrain approximation is reasonable for the present area of oil sands development, then an existing ADOE Gaussian model should be modified to include site-specific dispersion parameters.

There is considerable concern arising from studies in the Sudbury region that highly convective situations may be the worst meteorological conditions for very tall stacks and that most dispersion coefficients based upon surface layer experiments are inapplicable (Venkatram, personal communication, Ontario Ministry of Environment, 1979). The existing AOSERP data base may not be adequate to resolve the problem; however, if very tall stacks are contemplated in a development scenario, then free convection simulation may be very important. It is recommended that this free convection work be reviewed to determine whether a problem exists in the AOSERP area, and if so, whether modified sigma parameters are adequate and how they can be estimated for inclusion into the ADOE Gaussian model.

7.3 TERRAIN MODELS

Terrain will be important in at least some parts of the AOSERP region (Stoney Mountain). It is recommended that a modified potential flow model be implemented as a readily useable management tool. The same revisions of stability class selection and development of site specific dispersion coefficients as for the Gaussian models should be undertaken. An Eulerian k-theory is recommended as a dispersion formulation for reasons discussed in Section 6. Effort should be directed toward minimizing the numerical dispersion effects while retaining a relatively inexpensive operating cost.

7.4 IMPORTANCE OF TERRAIN EFFECTS

The distribution of areas having significant terrain effects in the AOSERP region needs to be identified. The analysis would need to consider at least four specific areas:

1. The Athabasca River Valley;
2. The Gregoire Lake Stoney Mountain area;
3. The terrain between the projected Alsands plant and the projected townsite; and
4. The more distant terrain features such as the Birch Mountains.

A suggested procedure would be to compare available minisondes and pibal records with surface winds and possibly analyzed synoptic patterns. Numerical studies with terrain models would be of real assistance.

7.5 REPRESENTATIVE WIND DATA

In order to drive the air quality models for the set frequency distribution and long-term deposition applications, a valid wind data set is required. There is some concern over whether Mildred Lake winds are representative of the winds determining pollutant dispersion from the main stacks. Analysis similar to that outlined above, for resolving terrain effects, is required. A procedure for generating a representative wind set may need to be developed if systematic discrepancies exist.

8. CONCLUSIONS

The conclusions of this review study of user needs and air quality simulation models are listed below:

1. The model selection procedure developed for this study involved application, implementation, and importance parameters to characterize the model types. This approach ensured a systematic consideration of the many factors involved in the selection of a recommended model. The use of the model selection procedure was complicated by the fact that the parameter values were functions of the user needs; since each identified user need did not necessarily require the simulation of all of the various physical processes that contributed to the application and implementation parameter values.
2. The interviews of potential users led to the identification of five user needs, of which three appeared to be of particular concern to AOSERP. These were: (1) the maintenance of air quality regulatory standards; (2) the generation of frequency distributions of canopy-top pollutant concentrations as functions of biologically important stratification parameters (such as surface moisture, temperatures, time of day, etc.); and (3) the long-term dry deposition patterns.
3. A number of air quality model types were recommended for meeting the identified user needs. In flat terrain, Gaussian models were considered adequate. In complex terrain, modified potential flow type models combined with a k-theory formulation were recommended. If flow separation phenomena are important, then a model incorporating momentum and, perhaps, energy conservation equations may be required.
4. The major disadvantage of interpolating flow models was identified as the continuing problem of obtaining statistically representative and sufficiently detailed wind data to drive the models.

5. The major disadvantage to the particle-in-cell dispersion formulations was identified as high computer costs.
6. Specific identified user needs required the accurate simulation of flow and dispersion features for only a limited number of meteorological situations or only after averaging over many realizations. For these specific identified model applications, simplified unidirectional wind profiles were considered acceptable as an input boundary condition and the numerical dispersion effects, often associated with Eulerian grid advection-diffusion formulations, were of less significance.
7. Specific stages of a model implementation program were outlined. These included: (1) the implementation of a Gaussian frequency distribution model of a modified CRSTER form to include site specific dispersion parameters and biological stratification parameters; (2) the site-tuning of a Gaussian standards model with a consideration of convective effects for tall stacks; (3) the implementation of a modified potential flow terrain model with site-specific dispersion coefficients; (4) the determination of the spatial distribution the importance of terrain effects in the AOSERP region; and (5) the generation of a representative wind data base for the frequency distribution model.

Finally, it should be emphasized that air quality models are tools and that the results obtained from the application of any tool are functions of both the quality of the tool and the experience of the craftsman. Even in routine operations, a trained air quality meteorologist/engineer is required to run the models. In complex terrain or complex meteorological situations where model capabilities are being pushed to their limits, a dispersion meteorologist is required to ensure proper application of the model and recognition of the limits of the reliability of the results.

9. REFERENCES CITED

Bass, A. and S.A. Orszag. 1976. Spectral modeling of atmospheric flows and turbulent diffusion. National Tech. Infor. Service, U.S. Dept., of Commerce, Springfield, Virginia. Report PB-252 506. 139 pp.

Batchelor, G.K. 1967. An introduction to fluid dynamics. Cambridge University Press, Cambridge, U.K. 615 pp.

Berkowicz, R. and L.P. Prahm. 1979. Generalization of k-theory for turbulent diffusion. Part I. Spectral turbulent diffusivity concept. JAM 36:266-272.

Briggs, G. 1975. Plume rise predictions. Pages 59-111 in D.A. Haugen, ed. Lectures on Air Pollution and Environment Impact Analyses. Amer. Met. Soc., Boston.

Bronwell, A. 1953. Advanced mathematics in physics and engineering. McGraw-Hill, New York. 475 pp.

Busch, N. E. 1973. On the mechanics of atmospheric turbulence. Pages 1-65 in D.A. Haugen, ed. Workshop on Micrometeorology. Amer. Met. Soc., Boston.

Christensen, O. and L.P. Prahm. 1976. A pseudospectral model for dispersion of atmospheric pollutants. JAM 15:1284-1294.

Davison, D.S. and K.L. Grandia. 1978. Plume dispersion measurements from an oil sands extraction plant, June 1977. Prep. for Alberta Oil Sands Environmental Research Program by Intera. AOSERP Report 52. 194 pp.

Davison, D.S. and E.D. Leavitt. 1979. Analysis of AOSERP plume sigma data. Prep. for Alberta Oil Sands Environmental Research Program by Intera. AOSERP Report 63. 251 pp.

Deardorff, J.W. 1973. Three-dimensional numerical modeling of the planetary boundary layer. Pages 271-311 in D.A. Haugen, ed. Workshop on Micrometeorology. Amer. Met. Soc., Boston.

Egan, B.A. 1975. Turbulent diffusion in complex terrain. Pages 112-135 in D.A. Haugen, ed. Lectures on Air Pollution and Environmental Impact Analyses. Amer. Met. Soc., Boston.

Eschenroeder, A.Q., J. Martinex, and R.A. Nordsiek. 1972. Evaluation of a diffusion model for photochemical smog simulation. USEPA Contract No. 68-02-0336.

Gifford, F.A. 1975. Atmospheric dispersion models for environmental pollution applications. Pages in D.A. Haugen, ed. Lectures on Air Pollution and Environmental Impact Analyses. Amer. Met. Soc., Boston.

Hanna, S.R., T.V. Crawford, W.B. Bendel, J.W. Deardorff, T.W. Horst, G.H. Fichtl, D. Randerson, S.P.S. Arya, J.M. Norman, and F.A. Gifford. 1977. Accuracy of dispersion models - a position paper of the AMS 1977 Committee on Atmospheric Turbulence and Diffusion. Bull. Amer. Met. Soc. 59(8):1025-1026.

Hino, M. 1968. Computer experiment on smoke diffusion over a complicated topography. Atm. Env. 2:541-558.

International Environmental Consultants Ltd. 1975. Comparative study of atmospheric dispersion models. CPAR Project Report 444-1. Distributed by CPAR Secretariat, Can. Forestry Service, Ottawa. 168 pp.

Islitzer, N.F. and D.H. Slade. 1968. Diffusion and transport experiments. Pages 117-188 in D.H. Slade, ed. Meteorology and atomic energy 1968. Prep. for U.S. Atomic Energy Comm. Available as TID-24190 NTIS, Springfield, Virgina.

Kumar, A. 1978. Pollutant dispersion in the planetary boundary layer. Syncrude Canada Ltd. Prof. Paper 1978-1.

Lamb, D.V., F.I. Badgley, and A.T. Rossano. 1973. A critical review of mathematical diffusion modeling techniques for predicting air quality with relation to motor vehicle transportation. Washington State Hwy. Dept. Research Program. Report 12.1.

Lange, R. 1978. ADPIC: a three-dimensional particle-in-cell model for the dispersal of atmospheric pollutants and its comparison to regional tracer studies. JAM 17:320-329.

Lantz, R.B., R.C. McCulloch, and R.K. Agrawal. 1972. The use of three-dimensional numerical air pollution models in planning plant location, design, and operation. J. Can. Petrol. Technol. 11:18-25.

Liu, M.K. and J.H. Seinfield. 1975. On the validity of grid and trajectory models of urban air pollution. Atm. Env. 9:555-696.

Long, P.E. and D.W. Pepper. 1976. A comparison of six numerical schemes for calculating the advection of atmospheric pollution. Preprints of 3rd Symposium on Atm. Turb. Diff. and Air Quality, Oct. 1976. Amer. Met. Soc., Boston, Mass. p. 181-187.

Monin, A. S. 1965. Structure of an atmospheric boundary layer. IZV. ANSSSR, Ser. Atm. and Oceanic Phys. 1(3):258.

Morris, R. and H.H. Slater. 1974. Modified rollback models. Proc. of 5th meeting of expert panel on air pollution modeling, NATO/CCMS, August 1974.

Padro, J. 1977. Review of dispersion models and possible applications in the AOSERP study area. Prep. for Alberta Oil Sands Environmental Research Program by Atmospheric Environment Service. AOSERP Project ME 4.2.1. 59 pp.

Pasquill, F. 1974. Atmospheric diffusion. Ellis Horwood. Chichester, U.K. 429 pp.

Pasquill, F. 1976. Atmospheric dispersion parameters in Gaussian plume modelling. Part II. Possible requirements for change in the Turner Workbook values. U.S. EPA Report EPA -600/4-76-030b. Research Triangle Park, North Carolina. 12 pp.

Prahm, L.P., R. Berkowicz, and O. Christensen. 1979. Generalization of k-theory for turbulent diffusion. Part II. Spectral diffusivity model for plume dispersion. JAM 36:273-282.

Prahm, L.P. and R. Berkowicz. 1979. Experimental evidence of predictions from the spectral turbulent diffusivity theory. Atmospheric Environment Service.

Reid, J.D., J.L. Walmsley, I.B. Findleton, and A.D. Christie. 1978. An assessment of the models LIRAQ and ADPIC for application to the Alberta Oil Sands Area. Prep. for Alberta Oil Sands Environmental Research Program by Atmospheric Environment Service. AOSERP Report 66. 95 pp.

Rote, D.M. 1976. Current uses and requirements for air quality models, a preliminary report. Prepared for NATO/CCMS Expert Panel on Air Quality Simulation Modeling. Argonne National Lab., Argonne, Illinois. 137 pp.

Runca, E. and F. Sardie. 1974. Numerical treatment of time dependent advection and diffusion of air pollutants. Atmospheric Environment Service. 9:69-80.

Sklarew, R.C., A.J. Fabrick, and J.E. Prager. 1971. A particle-in-cell method for numerical solution of the atmospheric diffusion equation, and applications to air pollution problems. Prep. for USEPA, available from NTIS as PB-209-29, Springfield, Virginia. 163 pp.

Slawson, P.R., G.A. Davidson, and C.S. Maddukuri. 1979. Dispersion modeling on the GCOS plume. Prep. for Syncrude Canada Ltd., May 1979. 268 pp.

Sutton, O.G. 1953. Micrometeorology. McGraw Hill, New York. 333 pp.

Tennekes, H. and J.L. Lumley. 1972. A first course in turbulence. MIT, Cambridge, Mass. 300 pp.

USEPA. 1978. Workbook for comparison of air quality models. Report No. EPA-450/2-78-0282. USEPA, Research Triangle Park, N.C., 104 pp.

Wyngaard, J.C. and O.R. Cote. 1974. The evolution of a convective planetary boundary layer--a higher-order-closure model study. BLM 7:289-308.

10. APPENDIX

10.1 PERSONS INTERVIEWED FOR THIS STUDY

The interviews conducted as part of this study were governed by several objectives. The primary objective was to assess real identifiable user needs in terms of what physical processes needed to be simulated in a numerical air pollution model. Another objective was to clarify the nature of the physical processes themselves in terms of the various ways in which they could be simulated in a model. The experience of other groups was sought through telephone interviews, in model selection methodology, and in the types of models that have proven to be useful.

The interviews all consisted of interactive discussions. Some users had not clearly identified exactly what their needs were in the context of simulation models. For example, the definition of space and time scales of interest involved questions of resolution, of absolute accuracy, of relative accuracy compared to neighbouring areas, of the various possible types of averaging, and of many other factors. Some users were not fully aware of the types of accuracy that are attainable with various models and types of averaging. The AMS Position Paper on the accuracy of dispersion models (Hanna et al. 1977) was presented frequently during the interviews to emphasize the attainable accuracies. Very often, a description of a particular user need emerged only after considerable discussion. For this reason, a questionnaire approach was not used.

A list of those individuals interviewed for this study is presented below in chronological order of the interviews. The objective in the selection of interviewers was to obtain a representative cross-section and not a complete and comprehensive list of all those working on or having an interest in environmental problems in the AOSERP region.

Mr. A. Mann	AOSERP, Air System Manager
Mr. R. Angle	Alberta Department of Environment
Dr. R. Seidner	AOSERP, Water System Manager
Dr. K. Hage	Meteorology Department, University of Alberta
Dr. J. Reid	Atmospheric Environment Service, Downsview
Dr. A. Venkatram	Ontario Ministry of Environment, Toronto
Dr. A. Christie	Atmospheric Environment Service, Downsview
Dr. T. Turner	Atmospheric Environment Service, Downsview
Dr. J. Walmsley	Atmospheric Environment Service, Downsview
Dr. C. Mathias	Atmospheric Environment Service, Downsview
Mr. S. Djurfors	Syncrude Canada Ltd.
Mr. R. Fesserden	Syncrude Canada Ltd.
Dr. A. Kumar	Syncrude Canada Ltd.
Dr. D. Netterville	Syncrude Canada Ltd.
Dr. D. Rote	Argonne National Laboratory, Chicago
Dr. C. D. Sapp	Air Quality Research Section, TVA, Alabama
Dr. H. Jones	Air Quality Research Section, TVA, Alabama
Dr. P. Addison	Canadian Forestry Service, Edmonton
Dr. S. Malhotra	Canadian Forestry Service, Edmonton
Dr. L. Barrie	Atmospheric Environment Service, Downsview
Mr. W. Cary	Great Canadian Oil Sands Ltd.
Mr. R. Wood	Great Canadian Oil Sands Ltd.
Dr. D. Balsillie	Ontario Ministry of Environment, Sudbury
Dr. A. Legge	Kananaskis Environmental Science Centre
Mr. S. Dobko	Alberta Department of Environment
Dr. S. Smith	AOSERP, Director
Mr. G. Young	N.E. Commissioner's Office
Dr. H. Sandhu	Alberta Department of Environment
Dr. C. Neill	Northwest Hydraulics Ltd., Edmonton
Dr. A. Khan	AOSERP, Land System Manager
Dr. A. Loman	Loman and Associates, Calgary
Dr. D. Whitfield	Botany Department, University of Alberta

11. LIST OF AOSERP RESEARCH REPORTS

1.		AOSERP First Annual Report, 1975
2.	AF 4.1.1	Walleye and Goldeye Fisheries Investigations in the Peace-Athabasca Delta--1975
3.	HE 1.1.1	Structure of a Traditional Baseline Data System
4.	VE 2.2	A Preliminary Vegetation Survey of the Alberta Oil Sands Environmental Research Program Study Area
5.	HY 3.1	The Evaluation of Wastewaters from an Oil Sand Extraction Plant
6.		Housing for the North--The Stackwall System
7.	AF 3.1.1	A Synopsis of the Physical and Biological Limnology and Fisheries Programs within the Alberta Oil Sands Area
8.	AF 1.2.1	The Impact of Saline Waters upon Freshwater Biota (A Literature Review and Bibliography)
9.	ME 3.3	Preliminary Investigations into the Magnitude of Fog Occurrence and Associated Problems in the Oil Sands Area
10.	HE 2.1	Development of a Research Design Related to Archaeological Studies in the Athabasca Oil Sands Area
11.	AF 2.2.1	Life Cycles of Some Common Aquatic Insects of the Athabasca River, Alberta
12.	ME 1.7	Very High Resolution Meteorological Satellite Study of Oil Sands Weather: "A Feasibility Study"
13.	ME 2.3.1	Plume Dispersion Measurements from an Oil Sands Extraction Plant, March 1976
14.		
15.	ME 3.4	A Climatology of Low Level Air Trajectories in the Alberta Oil Sands Area
16.	ME 1.6	The Feasibility of a Weather Radar near Fort McMurray, Alberta
17.	AF 2.1.1	A Survey of Baseline Levels of Contaminants in Aquatic Biota of the AOSERP Study Area
18.	HY 1.1	Interim Compilation of Stream Gauging Data to December 1976 for the Alberta Oil Sands Environmental Research Program
19.	ME 4.1	Calculations of Annual Averaged Sulphur Dioxide Concentrations at Ground Level in the AOSERP Study Area
20.	HY 3.1.1	Characterization of Organic Constituents in Waters and Wastewaters of the Athabasca Oil Sands Mining Area
21.		AOSERP Second Annual Report, 1976-77
22.		Alberta Oil Sands Environmental Research Program Interim Report to 1978 covering the period April 1975 to November 1978
23.	AF 1.1.2	Acute Lethality of Mine Depressurization Water on Trout Perch and Rainbow Trout
24.	ME 1.5.2	Air System Winter Field Study in the AOSERP Study Area, February 1977.
25.	ME 3.5.1	Review of Pollutant Transformation Processes Relevant to the Alberta Oil Sands Area

26.	AF 4.5.1	Interim Report on an Intensive Study of the Fish Fauna of the Muskeg River Watershed of Northeastern Alberta
27.	ME 1.5.1	Meteorology and Air Quality Winter Field Study in the AOSERP Study Area, March 1976
28.	VE 2.1	Interim Report on a Soils Inventory in the Athabasca Oil Sands Area
29.	ME 2.2	An Inventory System for Atmospheric Emissions in the AOSERP Study Area
30.	ME 2.1	Ambient Air Quality in the AOSERP Study Area, 1977
31.	VE 2.3	Ecological Habitat Mapping of the AOSERP Study Area: Phase I
32.		AOSERP Third Annual Report, 1977-78
33.	TF 1.2	Relationships Between Habitats, Forages, and Carrying Capacity of Moose Range in northern Alberta. Part I: Moose Preferences for Habitat Strata and Forages.
34.	HY 2.4	Heavy Metals in Bottom Sediments of the Mainstem Athabasca River System in the AOSERP Study Area
35.	AF 4.9.1	The Effects of Sedimentation on the Aquatic Biota
36.	AF 4.8.1	Fall Fisheries Investigations in the Athabasca and Clearwater Rivers Upstream of Fort McMurray: Volume I
37.	HE 2.2.2	Community Studies: Fort McMurray, Anzac, Fort MacKay
38.	VE 7.1.1	Techniques for the Control of Small Mammals: A Review
39.	ME 1.0	The Climatology of the Alberta Oil Sands Environmental Research Program Study Area
40.	WS 3.3	Mixing Characteristics of the Athabasca River below Fort McMurray - Winter Conditions
41.	AF 3.5.1	Acute and Chronic Toxicity of Vanadium to Fish
42.	TF 1.1.4	Analysis of Fur Production Records for Registered Traplines in the AOSERP Study Area, 1970-75
43.	TF 6.1	A Socioeconomic Evaluation of the Recreational Fish and Wildlife Resources in Alberta, with Particular Reference to the AOSERP Study Area. Volume I: Summary and Conclusions
44.	VE 3.1	Interim Report on Symptomology and Threshold Levels of Air Pollutant Injury to Vegetation, 1975 to 1978
45.	VE 3.3	Interim Report on Physiology and Mechanisms of Air-Borne Pollutant Injury to Vegetation, 1975 to 1978
46.	VE 3.4	Interim Report on Ecological Benchmarking and Biomonitoring for Detection of Air-Borne Pollutant Effects on Vegetation and Soils, 1975 to 1978.
47.	TF 1.1.1	A Visibility Bias Model for Aerial Surveys for Moose on the AOSERP Study Area
48.	HG 1.1	Interim Report on a Hydrogeological Investigation of the Muskeg River Basin, Alberta
49.	WS 1.3.3	The Ecology of Macrobenthic Invertebrate Communities in Hartley Creek, Northeastern Alberta
50.	ME 3.6	Literature Review on Pollution Deposition Processes
51.	HY 1.3	Interim Compilation of 1976 Suspended Sediment Date in the AOSERP Study Area
52.	ME 2.3.2	Plume Dispersion Measurements from an Oil Sands Extraction Plan, June 1977

53.	HY 3.1.2	Baseline States of Organic Constituents in the Athabasca River System Upstream of Fort McMurray
54.	WS 2.3	A Preliminary Study of Chemical and Microbial Characteristics of the Athabasca River in the Athabasca Oil Sands Area of Northeastern Alberta
55.	HY 2.6	Microbial Populations in the Athabasca River
56.	AF 3.2.1	The Acute Toxicity of Saline Groundwater and of Vanadium to Fish and Aquatic Invertebrates
57.	LS 2.3.1	Ecological Habitat Mapping of the AOSERP Study Area (Supplement): Phase I
58.	AF 2.0.2	Interim Report on Ecological Studies on the Lower Trophic Levels of Muskeg Rivers Within the Alberta Oil Sands Environmental Research Program Study Area
59.	TF 3.1	Semi-Aquatic Mammals: Annotated Bibliography
60.	WS 1.1.1	Synthesis of Surface Water Hydrology
61.	AF 4.5.2	An Intensive Study of the Fish Fauna of the Steepbank River Watershed of Northeastern Alberta
62.	TF 5.1	Amphibians and Reptiles in the AOSERP Study Area
63.	ME 3.8.3	Analysis of AOSERP Plume Sigma Data
64.	LS 21.6.1	A Review and Assessment of the Baseline Data Relevant to the Impacts of Oil Sands Development on Large Mammals in the AOSERP Study Area
65.	LS 21.6.2	A Review and Assessment of the Baseline Data Relevant to the Impacts of Oil Sands Development on Black Bears in the AOSERP Study Area
66.	AS 4.3.2	An Assessment of the Models LIRAQ and ADPIC for Application to the Athabasca Oil Sands Area
67.	WS 1.3.2	Aquatic Biological Investigations of the Muskeg River Watershed
68.	AS 1.5.3 AS 3.5.2	Air System Summer Field Study in the AOSERP Study Area, June 1977
69.	HS 40.1	Native Employment Patterns in Alberta's Athabasca Oil Sands Region
70.	LS 28.1.2	An Interim Report on the Insectivorous Animals in the AOSERP Study Area
71.	HY 2.2	Lake Acidification Potential in the Alberta Oil Sands Environmental Research Program Study Area
72.	LS 7.1.2	The Ecology of Five Major Species of Small Mammals in the AOSERP Study Area: A Review
73.	LS 23.2	Distribution, Abundance and Habitat Associations of Beavers, Muskrats, Mink and River Otters in the AOSERP Study Area, Northeastern Alberta
74.	AS 4.5	Air Quality Modelling and User Needs
75.	WS 1.3.4	Interim Report on a Comparative Study of Benthic Algal Primary Productivity in the AOSERP Study Area
76.	AF 4.5.1	An Intensive Study of the Fish Fauna of the Muskeg River Watershed of Northeastern Alberta
77.	HS 20.1	Overview of Local Economic Development in the Athabasca Oil Sands Region Since 1961.
78.	LS 22.1.1	Habitat Relationships and Management of Terrestrial Birds in Northeastern Alberta

79.	AF 3.6.1	The Multiple Toxicity of Vanadium, Nickel, and Phenol to Fish.
80.	HS 10.2 & HS 10.1	History of the Athabasca Oil Sands Region, 1980 to 1960's. Volumes I and II.
81.	LS 22.1.2	Species Distribution and Habitat Relationships of Waterfowl in Northeastern Alberta.
82.	LS 22.2	Breeding Distribution and Behaviour of the White Pelican in the Athabasca Oil Sands Area.
83.	LS 22.2	The Distribution, Foraging Behaviour, and Allied Activities of the White Pelican in the Athabasca Oil Sands Area.
84.	WS 1.6.1	Investigations of the Spring Spawning Fish Populations in the Athabasca and Clearwater Rivers Upstream from Fort McMurray; Volume I.
85.	HY 2.5	An intensive Surface Water Quality Study of the Muskeg River Watershed. Volume I: Water Chemistry.
86.	AS 3.7	An Observational Study of Fog in the AOSERP Study Area.
87.	WS 2.2	Hydrogeological Investigation of Muskeg River Basin, Alberta
88.	AF 2.0.1	Ecological Studies of the Aquatic Invertebrates of the Alberta Oil Sands Environmental Research Program Study Area of Northeastern Alberta
89.	AF 4.3.2	Fishery Resources of the Athabasca River Downstream of Fort McMurray, Alberta. Volume 1
90.	AS 3.2	A Wintertime Investigation of the Deposition of Pollutants around an Isolated Power Plant in Northern Alberta
91.	LS 5.2	Characterization of Stored Peat in the Alberta Oil Sands Area
92.	WS 1.6.2	Fisheries and Habitat Investigations of Tributary Streams in the Southern Portion of the AOSERP Study Area. Volume I: Summary and Conclusions
93.	WS 1.3.1	Fisheries and Aquatic Habitat Investigations in the MacKay River Watershed of Northeastern Alberta
94.	WS 1.4.1	A Fisheries and Water Quality Survey of Ten Lakes in the Richardson Tower Area, Northeastern Alberta. Volume I: Methodology, Summary, and Discussion.
95.	AS 4.2.6	Evaluation of the Effects of Convection on Plume Behaviour in the AOSERP Study Area
96.	HS 20.3	Service Delivery in the Athabasca Oil Sands Region Since 1961
97.	LS 3.4.1	Differences in the Composition of Soils Under Open and Canopy Conditions at Two Sites Close-in to the Great Canadian Oil Sands Operation, Fort McMurray, Alberta
98.	LS 3.4.2	Baseline Condition of Jack Pine Biomonitoring Plots in the Athabasca Oil Sands Area; 1976 and 1977
99.	LS 10.1	Synecology and Autecology of Boreal Forest Vegetation in the AOSERP Study Area
100.	LS 10.2	Baseline Inventory of Aquatic Macrophyte Species Distribution in the AOSERP Study Area
101.	LS 21.1.3	Woodland Caribou Population Dynamics in Northeastern Alberta
102.	LS 21.1.4	Wolf Population Dynamics and Prey Relationships in Northeastern Alberta