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INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM) PHASE 1 REPORT: INTERIM RECOMMENDATION FOR MODELING LONG RANGE TRANSPORT AND IMPACTS ON REGIONAL VISIBILITY

Office of Air Quality Planning and Standards
Clean Air
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INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM) PHASE 1 REPORT: INTERIM RECOMMENDATION FOR MODELING LONG RANGE TRANSPORT AND IMPACTS ON REGIONAL VISIBILITY

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FORWARD

This document is being released as a publication of the Environmental Protection Agency (EPA) in response to a request from members of the Interagency Workgroup on Air Quality Modeling (IWAQM). Members include representatives from the Environmental Protection Agency, U.S. Forest Service, National Park Service, and U.S. Fish and Wildlife Service. The document includes recommendations on how to estimate air quality impacts associated with prevention of significant deterioration due to sources farther than 50 km from a Class I area. Impacts on visibility and other air quality related values at all downwind distances are also addressed. IWAQM recommends that the MESOPUFF-II model be used for these analyses in a somewhat different mode than previously suggested by EPA.

The recommendations of IWAQM contained in this document should be considered interim until more suitable techniques can be developed and tested. Implementation of these recommendations is a matter for the appropriate regulatory agencies and should be done in consultation with the applicable EPA Regional Office.

PREFACE

The Interagency Workgroup on Air Quality Modeling (IWAQM) was formed to provide a focus for development of technically sound, regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. Meetings were held with personnel from interested Federal agencies, viz. the Environmental Protection Agency, the U.S. Forest Service, the National Park Service, and the U.S. Fish and Wildlife Service. The purpose of these meetings was to review respective regional modeling programs, to develop an organizational framework, and to formulate reasonable objectives and plans that could be presented to management for support and commitment. The members prepared a memorandum of understanding (MOU) that incorporated the goals and objectives of the workgroup and obtained signatures of management officials in each participating agency. Although no States are signatories, their participation in IWAQM functions is explicitly noted in the MOU.

This Phase 1 Report is published by the IWAQM in an effort to provide the sponsoring agencies and other interested parties information on appropriate "off-the-shelf" methods for estimating long range transport impacts of air pollutants on Federal Class I areas and impacts on regional visibility. The IWAQM members anticipate issuing additional publications related to progress toward meeting the IWAQM goals and objectives, the results of model evaluation studies, proposed and final recommendations on modeling systems for regulatory applications, and other topics related to specific objectives in the MOU.

ACKNOWLEDGEMENTS

The members of the IWAQM acknowledge the special efforts of John Vimont of the National Park Service for composing the contents of this document and conducting most of the technical work. The IWAQM would also like to acknowledge Alan Cimorelli and John Irwin of the U.S. Environmental Protection Agency; Richard Fisher of the U.S. Forest Service; Elwyn Rolofson of the U.S. Fish and Wildlife Service; Patrick Hanrahan of the State of Oregon, Department of Environmental Quality; Kenneth McBee and James Browder of the Commonwealth of Virginia, Department of Air Pollution Control; and Mark Scruggs of the National Park Service for their input and suggestions on assembling this document and their subsequent review. IWAQM also thanks Brenda Cannady for her help in preparing and proofreading the final text.

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EXECUTIVE SUMMARY

The need for a consistent, technically credible approach for evaluating the impacts of sources of air pollution located more than 50 kilometers from Class I wilderness areas and national parks, on those areas, has been identified. The Interagency Workgroup on Air Quality Modeling (IWAQM), consisting of representatives from the agencies responsible for managing the wilderness and national park resources [the U.S. Forest Service (USFS), the National Park Service (NPS), and the U.S. Fish and Wildlife Service (FWS)], and the Environmental Protection Agency (EPA), was formed to develop regional analysis techniques to evaluate such impacts. The major charge of the IWAQM is to develop a modeling approach for the permitting of new and modified air pollution sources which impact these Federal Class I areas. To this end the IWAQM has developed a multi-year workplan (EPA, 1992) which is to be implemented in three phases. Recognizing the immediate need within the permitting community, the first phase of the workplan called for an interim recommendation, by October of 1992. Given the time constraints and the practical limitations of resources and hardware, Phase 1 was designed to provide the best approach from existing "off-the-shelf-techniques." This report documents the work performed and conclusions reached in support of the Phase 1 recommendation (stated below). Therefore, the IWAQM is proposing a technique, which will satisfy the above listed need, to be used in the interim, until a more refined technique is recommended in Phase 2. The recommended Phase 1 approach is to use the Lagrangian puff model, MESOPUFF-II (Scire *et al.*, 1984b), to evaluate the impacts of pollutants from sources located more than 50 kilometers from Class I areas, up to several hundred kilometers from Class I areas. The impacts of concern are the allowable Class I increases in pollutants (increments), the National

Ambient Air Quality Standards (NAAQS), and Air Quality Related Values (AQRVs). AQRV impacts include such effects as visibility degradation and acidic deposition. The recommended modeling technique is suitable for conducting single source impact analyses, as well as, cumulative impact analyses. The results from this technique will frequently need to be combined with the results from techniques used to estimate concentrations from sources closer than 50 kilometers to a receptor area.

It is important to note that by restricting the models considered for Phase 1 to "off-the-shelf" techniques, the IWAQM recognizes certain limitations in the suggested techniques. These include limits in considering the effects of terrain on the long range transport and dispersion, an underestimation of the conversion of SO_2 to $SO_4^=$ when polluted air interacts with clouds, and an overestimation of particulate nitrate when a limited number of sources is considered. Furthermore, the estimations of the impacts of sources on regional visibility are simple and do not account for all of the processes important to regional visibility. Nonetheless, the IWAQM considers the techniques, suggested herein, to be a significant improvement over those previously used, in that previous techniques ignored many of the processes important to the assessment of air quality impacts in Class I areas. Under some circumstances, the concentrations of sulfates in the atmosphere may be underestimated, and hence the impacts on regional visibility, due to the inability of the model to treat in-cloud processes. The IWAQM, including the representatives of the land management agencies, recognize these limitations and consider the suggested techniques to be technically superior to simply assuming that there are no impacts on regional visibility. As the IWAQM work continues, these limitations will be addressed, to the extent possible.

The IWAQM assessed two models for this recommendation, the MESOPUFF-II model and the Acid Rain Mountain Mesoscale Model (ARM3). It was believed that the transport and dispersion portions of both models could be consistent with requirements outlined in the *Guideline on Air Quality Models (Revised)* (EPA, 1986). Upon careful examination of both models, however, coding errors were discovered in the ARM3, which potentially invalidated its previous evaluations. Therefore, the MESOPUFF-II is being recommended, since it satisfies requirements for Class I area evaluation.

The meteorological preprocessor which is used by the MESOPUFF-II model (MESOPAC) does not account for terrain influences on the wind field. Also, the IWAQM has shown that MESOPAC produces discontinuities in the mixing height field. The IWAQM has reasoned that the possible errors introduced by the shortcomings of MESOPAC are outweighed by the immediate need for the Phase 1 recommendation. Therefore, the recommendation, as stated below, is being made at this time. However, the IWAQM has identified an existing meteorological preprocessor which could be used, in place of MESOPAC. This preprocessor utilizes a technique for smoothing the mixing height fields and accounts for terrain through the use of a diagnostic wind model. It is the IWAQM's intention to revise the Phase 1 recommendation, to substitute this processor for MESOPAC, as soon as it has been adequately tested within the MESOPUFF II structure.

Recommendations for running the MESOPUFF-II model are provided for increment, NAAQS, and AQRV analyses. Methods are also provided for combining its results with the results from steady-state, Gaussian plume models, which are generally used for calculating impacts from sources closer than 50 kilometers from receptors. A technique for evaluating regional haze impacts from a single source or from a number of sources is also provided.

PHASE 1 RECOMMENDATION SUMMARY

Until the Phase 2 work of the IWAQM is complete the IWAQM recommends the following modeling approach be used under circumstances which require the analysis of Class I area impacts for sources more than 50 kilometers and up to several hundred kilometers away. This recommendation is interim in that certain technical compromises were made in order to satisfy the immediate need for a workable modeling approach.

I. LEVEL I ANALYSIS (PLUME MODEL)

A. PSD INCREMENT AND STANDARDS

(1) For conditions other than extended stagnation or known conditions of pollutant recirculation, a steady-state, Gaussian plume model may be used for all sources.

(2) Mass removal model options for either chemical transformation or deposition should not be employed.

(3) Where recirculation or stagnation is known to be important the applicant should use the Level II analysis only.

(4) If the Level I analysis indicates an exceedance then a complete Level II analysis should be performed.

B. VISIBILITY

The applicant should use the same approach as is described in I.A. with the following additions:

(1) Assume that all of the emitted SO_2 and NO_x has been converted to $SO_4^=$ and NO_3^- respectively.

(2) The concentrations of $SO_4^=$ and NO_3^- should then be used in conjunction with the techniques presented in Appendix B to estimate impacts on Class I area visibility.

C. OTHER AQRVs

The applicant should use the same approach as is described in I.A. with the following additions:

(1) Assume that all of the emitted SO_2 remains as SO_2 and that the NO_x has been converted to HNO_3.

(2) Use appropriate deposition velocities to estimate the deposition of the pollutants. (See Inset 2.)

II. LEVEL II ANALYSIS (MESOPUFF-II)

A. PSD INCREMENT AND STANDARDS

(1) For sources > 50 km (and up to several hundred km) from all Class I area receptors MESOPUFF-II should be used.

(2) For sources ≤ 50 km from all Class I area receptors, models recommended for use in the EPA Modeling Guideline should be used.

(3) For those sources located such that some Class I receptors are ≤ 50 km and others are > 50 km the applicant may either

 (a) model all receptors with a Guideline model, or

 (b) model those receptors which are > 50 km with MESOPUFF-II and those which are ≤ 50 km with a Guideline model.

(4) Concentrations from all sources should be summed hour-by-hour, receptor-by-receptor and pollutant-by-pollutant.

B. VISIBILITY

(1) All sources being analyzed, regardless of their distance from the Class I area, should be modeled with MESOPUFF-II following the procedures set forth in Appendix A.

(2) Using the predicted concentrations of $SO_4^=$ and NO_3^-, regional haze calculations should be made in accordance with the procedures set forth in Appendix B.

(3) If it is determined that plume blight analyses need to be made, the recommendations regarding use of VISCREEN and PLUVUE II in the *Guideline on Air Quality Models (Revised)* should be followed.

C. OTHER AQRVs (Depositional Loading)

(1) All sources being analyzed, regardless of their distance from the Class I area, should be modeled with MESOPUFF-II following the procedures set forth in Appendix A.

(2) Outputs of $SO_4^=$ and NO_3^- deposition should be used, as necessary, to quantify the impact to aquatic and terrestrial ecosystems. Close coordination with the Federal Land Manager will be necessary in determining the appropriate averaging times for this analysis.

III. MESOPUFF-II

The following applies to all applications of MESOPUFF II within the context of the Phase 1 recommendation.

A. Follow the recommendations found in Appendix A.

B. The cross over distance for the time dependent dispersion curves should be set to 10 km.

C. Both wet and dry deposition options should be employed.

D. The model's chemical transformation algorithms should be employed.

IV. METEOROLOGY

A. PERIOD OF RECORD (Applies to both MESOPUFF-II and Guideline models)

(1) A five year National Weather Service (NWS) meteorological data record should be used when the applicant source is either > 50 km from the Class I area or is within 50 km and does not have at least one year of on-site data.

(2) For an applicant source located within 50 km of a Class I area, all sources being modeled should use a representative data record which corresponds to the time period of the on-site data. On-site data can not be used unless it covers at least one full year. Furthermore, if more than one year of on-site data exists it should be used up to the most recent 5 years.

B. SELECTION OF DATA BASES

(1) GUIDELINE MODEL: It may be desirable to divide the analysis domain into meteorologically similar areas and use area specific representative meteorological data to model all sources' impacts in that area. The use of multiple meteorological data bases is not the normal practice with Guideline models and should be approved on a case-by-case basis by the appropriate regulatory authority.

(2) MESOPUFF-II: The number and location of the NWS meteorological data bases to be used in the MESOPUFF-II analysis should be determined on a case-by-case basis, generally using all available, <u>representative</u> data.

1. INTRODUCTION

Under the Clean Air Act, special protection from adverse air quality impacts is afforded certain national parks and wilderness areas, through the Prevention of Significant Deterioration (PSD) program. These areas have been designated as Class I areas, and as such, increases of pollutant levels in these areas are strictly limited. Furthermore, the Federal Land Manager (FLM) of the Class I area is given an affirmative responsibility to ensure that Air Quality Related Values (AQRVs) are not adversely impacted. [The FLMs of the Class I areas are the U.S. Forest Service (USFS), the National Park Service (NPS), and the U.S. Fish and Wildlife Service (FWS).] Air quality models are one of the primary tools used to assess the impacts from sources of air pollution on both the established PSD increments and the AQRVs. Steady-state models are generally used for PSD analyses, however, as the PSD program has developed, the need for more sophisticated models to assess air quality impacts in Class I areas, from sources at relatively greater distances from the Class I areas, has arisen. In some areas, the FLMs have asserted that Class I areas have been adversely affected by air pollution and that new sources of pollution over a broad area are further harming the resource. The absence of any recommended long range modeling techniques has left permitting authorities without the means to assess the assertions of the FLMs. The Environmental Protection Agency (EPA) and the FLMs have undertaken various model development efforts to address the air quality impacts of pollution transported over relatively long distances. The Interagency Workgroup for Air Quality Modeling (IWAQM) was formed to coordinate the independent modeling efforts of the EPA and the FLMs so that a consistent, technically credible approach can be recommended and used.

The IWAQM work plan (EPA, 1992) describes a phased approach to satisfy the modeling needs described above. Phase 1 consists of reviewing EPA guidance and "off-the-shelf-technology" for recommending a modeling approach to meet the immediate need for a regional scale model for ongoing permitting activity. It is important to note that in order to satisfy this immediate need, the IWAQM restricted itself to "off-the-shelf-technology." Phase 1, described herein, is based on current EPA guidance and existing models, which have been further reviewed by the IWAQM. During Phase 2, the workgroup will augment Phase 1 with a review of other available models and make a recommendation of the most appropriate modeling techniques. The Phase 2 recommendation will represent a compromise between the current modeling state-of-science and best available operational computer capabilities. The IWAQM recognizes this later recommendation may change the initial, first phase, interim recommendation. More advanced modeling techniques will be considered in Phase 3.

Models used to evaluate the impact of sources of air pollution on the PSD increments and National Ambient Air Quality Standards (NAAQS), are required to follow the *Guideline on Air Quality Models (Revised)* (EPA, 1986). (Hereafter, referred to as the *Guideline*.) For many situations, preferred models, considered generally applicable under a variety of circumstances, are defined. When a physical situation exists for which there are no preferred models, criteria are established in the *Guideline* to use appropriate methods. These criteria are:

1. The model can be demonstrated to be applicable to the problem on a theoretical basis, and

2. the data bases which are necessary to perform the analysis are available and adequate, and

3a. performance evaluations of the model in similar circumstances have shown that the model is not biased toward underestimates, or

3b. after consultation with the EPA Regional Office, a second model is selected as a baseline or reference point for performance and the interim procedures are then used to demonstrate that the proposed model performs better than the reference model.

One such situation is long range transport, that is, transport of pollution beyond distances of 50 km. Therefore, in order for any Phase 1 recommendation to be viable, from a regulatory point of view, it will need to satisfy criteria 1., 2., and 3a. above. It is recognized that justification of an approach under 3b. is beyond the scope of most projects.

The processes which become important in the transport of pollution over long distances include the spatial and temporal variability of the winds which transport and disperse air pollutants in the presence of various terrain and water features, the chemical transformation of the pollutants as they travel, and the deposition of the pollutants along the way. There are existing long range transport models available which meet some, but not all of these needs and some which meet these needs, but have not been sufficiently tested.

One of the primary goals of the IWAQM is to evaluate existing modeling codes and either recommend one as an accepted approach or combine the better elements of several of the existing codes, creating a new modeling construct. Either of the above approaches will require full testing and evaluation. Creating a model with all of the desired features and testing it and evaluating it requires time. There is, however, an immediate need for assessing the impacts of long range transport of pollutants into Class I areas. Therefore, the IWAQM decided to review a limited set of existing long range transport models and recommend a specific model, which meets the *Guideline* criteria, for long range transport analysis, in the interim, until a more comprehensive solution can be formulated and tested. In addition to the recommendations of a specific long range transport model the Phase 1 recommendation also specifies how this model, in conjunction with existing regulatory models, should be used to provide those analyses necessary for Class I PSD permitting.

By restricting the models considered for Phase 1 to "off-the-shelf" techniques, the IWAQM recognizes certain limitations in the suggested techniques. These include a lack of consideration of the effects of terrain on the long range transport and dispersion, an underestimation of the conversion of SO_2 to $SO_4^{=}$ when polluted air interacts with clouds, and an overestimation of particulate nitrate when a limited number of sources are considered. Furthermore, the estimations of the impacts of sources on regional visibility are simple and do not account for all of the processes important to regional visibility. Nonetheless, the IWAQM considers the techniques, suggested herein, to be a significant improvement to those previously used, in that previous techniques ignored many of the processes important to the assessment of air quality impacts in Class I areas. Under some circumstances, the concentrations of sulfates in the atmosphere may be underestimated, and hence the impacts on regional visibility, due to the inability of the model to treat in-cloud processes. The IWAQM, including the representatives of the land management agencies, recognize these limitations and consider the suggested techniques to be technically superior to simply assuming that there are no impacts on regional visibility. As the IWAQM work continues, these limitations will be addressed, to the extent possible.

Two models were selected for consideration for an interim approach, the Acid Rain Mountain Mesoscale Model (ARM3) (Morris *et al.*, 1988) and the MESOPUFF-II model (Scire *et al.*, 1984b). The MESOPUFF-II model was considered by the EPA for inclusion in its list of refined models in the *Guideline*, but was subsequently suggested for inclusion only in Appendix B of the *Guideline*, the section reserved for models which could be considered for regulatory use, but not generically preferred. The NPS has been evaluating the ARM3 for use in its program of evaluating the impacts of air pollution in the national parks. As part of this evaluation, they chose to compare some of the ARM3 results against MESOPUFF-II because of MESOPUFF-II's availability and its consideration by the EPA. These two models both contain features considered desirable in a model for use in long range transport to Class I areas, particularly the ability to consider the chemical transformation of SO_2 and NO_X to $SO_4^=$ and NO_3^- and the removal of chemical species through deposition. In addition, the ARM3 contains algorithms for considering the effects of terrain on dispersion and on the transport flow. Furthermore, both of these models have been compared against other, similar models and have performed somewhat better than those other models relative to measured tracer data (Carhart *et al*., 1989; Moore *et al*., 1990).

The IWAQM recognizes that there are certain risks involved with recommending an interim long range modeling approach. From a regulatory perspective, it is generally desirable to use an interim model which will yield somewhat higher impact calculations than a more refined, preferred approach. In the case of steady-state air quality models for example, this can be relatively easily ensured because of the independence of the concentration calculations from one hour to the next. In the case of the Lagrangian long range transport models under consideration here, the concentration calculations for a given hour will be explicitly dependent on the spatially and temporally varying wind field from that hour and previous hours. Therefore, the exact behavior of a given modeling system relative to a similar but different modeling system can not be predicted with certainty.

2. EXISTING MODEL COMPARISONS AND EVALUATIONS

There have been a number of surveys of long range transport models which may be suitable for estimating the concentrations of pollutants which degrade visibility and/or contribute to acid deposition. One such survey (Thompson *et al.*, 1987) used a series of screenings and rankings to narrow the field of Lagrangian, Eulerian, hybrid, and statistical models which they would consider for application in western Canada. The model characteristics this study considered important were:

a. domain - 0 to 500 km and up to one year
b. resolution - 1 to 10 km and event to seasonal
c. predictands - ambient air concentrations of SO_2, $SO_4^=$, HF, metals, oxidants and NO_x
d. processes - convective and frontal storms, flow in complex terrain, rain and snow scavenging, influences of soil particles, cloud physics and chemistry
e. design - modular
f. accuracy - ±30 percent for sulfate concentration and deposition
g. chemistry - nonlinear.

The desire for a model which exhibits these characteristics is also shared by the IWAQM. A relatively small number of the potentially available models were identified through this process. The MESOPUFF-II model was among the models identified as meeting the criteria of the survey.

Another review of models was conducted for the EPA as part of the Rocky Mountain Acid Deposition Model Assessment (Morris and Kessler, 1987). The conclusion of this study was that "...no one meteorological or acid deposition model is significantly superior to the others; all the candidate models contained different features that would be desirable attributes in an acid deposition model for the Rocky Mountain region. Hence, the conceptual design of the mesoscale acid deposition model uses modules selected from various existing meteorological and acid deposition models." This ultimately lead to the development of the Acid Rain Mountain Mesoscale Model (ARM3).

While there have been a number of reviews and surveys of models and modeling features which could potentially address long range transport and visibility and acid deposition effects, there have been relatively few model evaluation efforts against field data. One such effort examined eight short-term, long-range transport models (Carhart *et al.*, 1989). The models were tested against two tracer data bases. One of the data bases was collected in Oklahoma from perfluorocarbon tracer releases upwind of sampling arcs placed at 100 and 600 km. The second data base was collected at the Savanna River Plant from the release of Kr^{85} gas from a 62 m stack. The samplers from this experiment were at distances from 28-144 km downwind. The main method used in the evaluation of the performance of the models was the application of the American Meteorological Society (AMS) Statistics. Additional statistics were added to the AMS recommended list in order to assist in interpreting the results. In addition, graphical analyses were used to supplement the statistical comparisons in order to shed light on the causes of model performance trends identified by the statistics. The data bases both involve an inert tracer, therefore, the evaluations only deal with the transport and dispersion algorithms of the models and not the deposition or chemical conversion algorithms. The field experiments were not designed to evaluate dispersion in complex terrain. Some of the important conclusions of this study were:

> The causes of model/data discrepancies can be largely traced to inadequate wind field modeling that leads to an incorrect temporal and spatial positioning of the plume, and the use of the Turner curves to downwind distances beyond which they can accurately represent the scales of atmospheric turbulence. The use of multilayer wind field models and the use of the Heffter formula for lateral plume dispersion close to the source appear to improve model accuracies.

The above model evaluation study was being conducted about the time that the Acid Rain Mountain Mesoscale Model (ARM3) was being completed. As the final portion of the Rocky Mountain Acid Deposition Model Assessment Project, the ARM3 was evaluated against the same data bases, using the same statistics. The results of that evaluation were that the overall performance of the ARM3 was similar to that of MESOPUFF-II (Moore *et al.*, 1990). Again, it should be noted that the data bases used in these analyses were not designed to stress the models' ability to simulate transport and dispersion in complex terrain.

The MESOPUFF-II model was also evaluated against data collected during the Cross-Appalachian Tracer Experiment (CAPTEX) (Godowitch, 1989). This experiment did include some transport and dispersion over complex terrain. This study concluded that any bias in the model estimates was toward over-prediction of measured concentrations.

3. CANDIDATE MODELS

For the interim recommendation, the IWAQM only considered models which could meet the *Guideline* criteria for the use of alternative models, described above. Due to the results of the above evaluations, the model features, the availability of the models, and the relative familiarity of the MESOPUFF-II model and the ARM3 to the IWAQM, these models seemed the logical choice to consider for this interim recommendation. The IWAQM considered that either model was applicable on a theoretical basis, that the available evaluation data bases, referred to above, are adequate, although not ideal for the purposes cited herein, and that the evaluations of the models indicated that there was not a systematic bias toward underestimation. While these models meet the *Guideline* criteria, the IWAQM recognizes that there are potentially other models which might be better suited for a particular application, but for general long range transport modeling, the aforementioned models should be adequate.

3.1 MESOPUFF-II

The following is an excerpt from the abstract of the *Development of the MESOPUFF-II Dispersion Model*, (Scire *et al.*, 1984a), which provides a good summary of the nature of and features of the MESOPUFF-II model:

> ...MESOPUFF-II is a Lagrangian variable-trajectory puff superposition model suitable for modeling the transport, diffusion and removal of air pollutants from multiple point and area sources at transport distances beyond the range of conventional straight-line Gaussian plume models (i.e., beyond ~ 10-50 km). It is an extensively modified version of the MESOscale PUFF (MESOPUFF) model (Benkley and Bass, 1979). Major additions and enhancements include: use of hourly surface meteorological data and twice-

daily rawinsonde data; separate wind fields to represent flow within and above the boundary layer; parameterization of vertical dispersion in terms of micrometeorological turbulence variables; parameterization of SO_2, to $SO_4^=$ and NO_x to NO_3^- conversion, including the chemical equilibrium of the $HNO_3/NH_3/NH_4NO_3$ system; resistance modeling of dry deposition, including options for source or surface depletion; time- and space-varying wet removal; and a computationally efficient puff sampling function...

One of the limitations of the model, with respect to the calculation of pollutant concentrations in Class I areas, which are frequently located in complex terrain areas, is the absence of any complex terrain treatment either on the generation of the meteorological fields or on the dispersion. The shortcoming of the meteorological fields is overcome to the extent that the meteorological observations, which are used to generate the wind fields in the MESOPAC meteorological processor, represent the influence of terrain. The lack of influence of complex terrain on the dispersion is somewhat obviated by the fact that at the downwind distances of the receptors from the sources, envisioned by the use of this model, the puff will generally be uniformly mixed throughout the depth of the mixed layer. Therefore, in most applications, it is not expected that these shortcomings will overwhelmingly bias the results of this model.

3.2 Acid Rain Mountain Mesoscale Model (ARM3)

The following brief description of the ARM3 is taken from the preface to the ARM3 users guide (Morris *et al.*, 1988):

...The ARM3 model is a Lagrangian trajectory model with simplified chemistry applied to the discrete plume parcels...

The ARM3 model consists of mesoscale meteorological modules and acid deposition/air quality modules applied to the plume parcels transported with the winds in the Lagrangian frame...

A three-dimensional diagnostic wind model is used to calculate the spatially and temporally varying wind fields. Kinematic, blocking and deflection, and thermodynamic effects are accounted for through simple parameterizations. The wind model is designed to generate wind fields within regions with sparse data; thus, the validity of the wind field is highly dependent on the quality of the observations and their applicability to the interpolation applied between the observations. Each interpolation of the observed temperature, dew point, and precipitation amounts contains an orographic adjustment based on limited climatological data from the Rocky Mountain region... Mixing height, stability classification, friction velocity, convective velocity, Monin-Obukhov length, and surface pressure are all estimated at each grid cell using appropriate algorithms with interpolated observations...

The acid deposition/air quality modules treat the plume parcels along their trajectories. The height of the parcel can be set either as terrain-following or reduced relative to the difference between the elevation of the terrain at the parcel location and elevation at the stack base...

There are three options for determining dispersion rates. The use of the Pasquill-Gifford dispersion rates provides the minimum dispersion. The other options provide higher dispersion rates that may be appropriate over regions of complex terrain. The dry deposition algorithm is based on the resistance approach. A dry deposition velocity is calculated based on the land-use type at the plume parcel location. The algorithm in the ARM3 is comparable to those in other models that use this approach. The wet deposition algorithm uses the scavenging coefficient approach. The precipitation rate for the grid cell containing the centroid of the Lagrangian parcel is used...

Chemical transformation of SO_2 and NO_2 to sulfate and nitrate can be calculated in the ARM3 using one of two highly-parameterized options in the ARM3 model. They are the methods adopted from the RIVAD [Regional Impact in Visibility and Acid Deposition Model] and the MESOPUFF-II models...

> To treat the aqueous-phase formation of sulfate, both mechanisms assume a linear oxidation rate that depends only on the SO_2 concentrations. RIVAD uses a constant rate of 0.2 percent/hr MESOPUFF uses a rate that ranges from 0.2 to 3 percent/hr depending on the relative humidity...

The ARM3 is of a similar nature to the MESOPUFF-II model, except that it has algorithms which explicitly treat complex terrain. These include a diagnostic wind model which treats kinematic and blocking effects of terrain on the air flow, dispersion parameters for complex terrain, and a correction for plume height as a plume passes over terrain. These enhancements should, ostensibly, make it more suitable for calculations in complex terrain.

3.3 Model Comparison and Further Technical Assessment

Rather than proceed with recommending a model strictly based upon its reported technical merits, a series of comparison runs were conducted to test the manner in which the models function under varying input conditions. The workgroup also examined the results of the meteorological processors of the two models under consideration, to appraise the credibility of the fields produced.

3.3.1 Initial Air Quality Model Comparisons

The first step undertaken was to run the ARM3 and MESOPUFF-II for a hypothetical point source located in south-central Virginia and calculate the concentrations of pollutants which might reach Shenandoah National Park. These analyses used available National Weather Service data for July 1984 (Figure 1). The results of these analyses were unexpected.

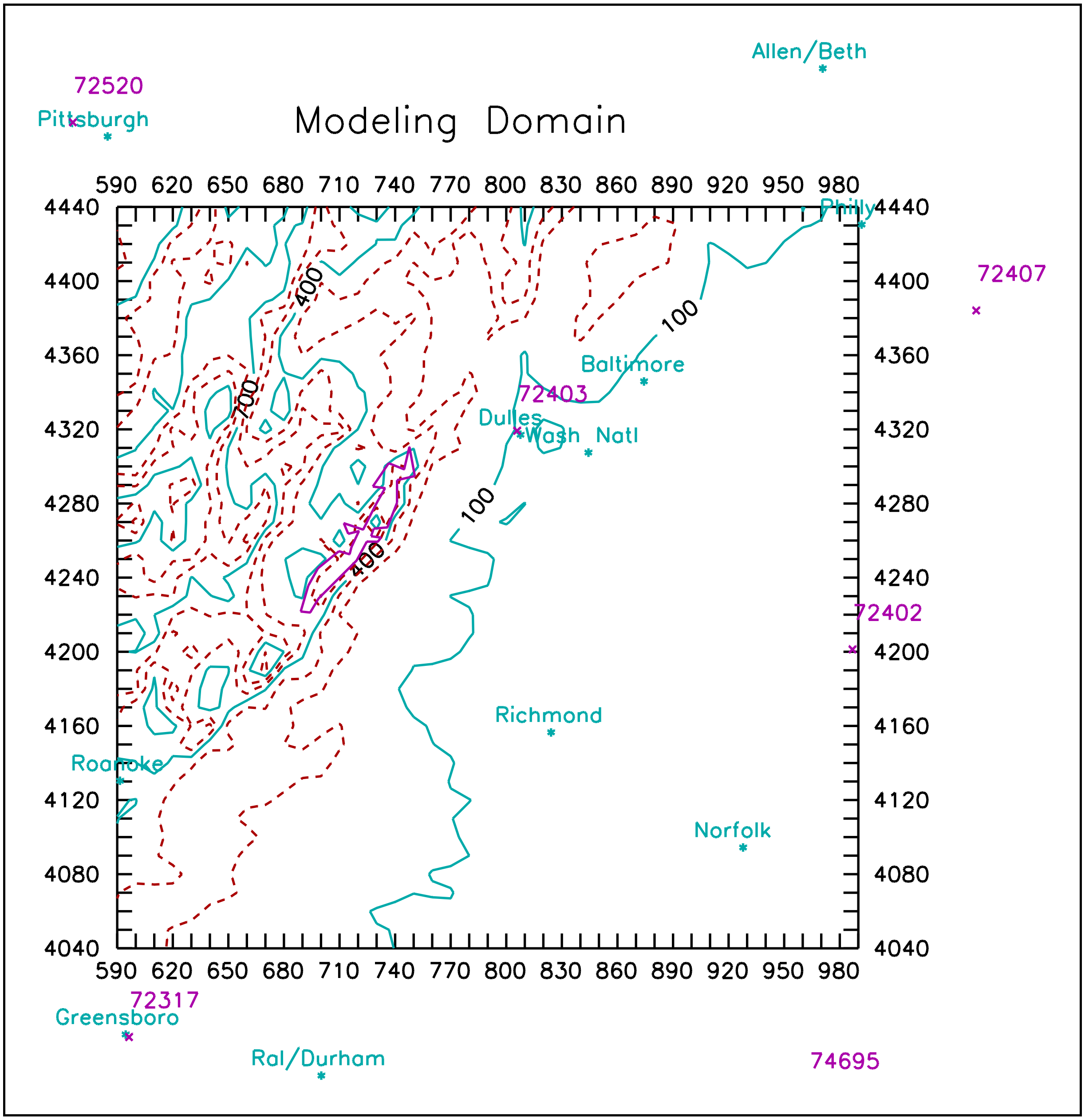

Figure 1 - Modeling domain used in comparison analysis. Surface meteorological stations are indicated by place name. Rawinsonde stations are indicated by station number. Elevations contours are in meters.

The concentrations of pollution calculated by the ARM3 were approximately an order of magnitude higher than those calculated using MESOPUFF-II. Since this result was not expected, the IWAQM undertook a series of model runs to determine whether some of the fundamental differences in the air quality model formulations were responsible for the dramatic concentration differences or whether differences in the generation of the meteorological fields were responsible.

First, both models were run in an inert mode; that is, the options for calculation of chemical transformation and deposition were turned off. The dissimilarities in results, were again, essentially the same. It was considered that differences in the results stemmed from the treatment of complex terrain in the ARM3, either in the wind fields or the plume dispersion and transport algorithms. Complex terrain potentially has two effects when considering concentration calculations from the ARM3 air quality model. First, under the options selected for this series of tests of ARM3, the dispersion of pollutants is enhanced by the effects of the complex terrain. The second effect was the influence terrain has on bringing the receptor closer to the plume elevation. The first effect would have a tendency to lower the concentration estimates, while the latter could potentially increase the concentration estimates. Therefore, it was decided to run the ARM3 without the plume height to receptor correction included on the original runs. The removal of this option had little effect on the concentrations calculated by the model; this was not the expected result. Furthermore, selecting the option within the ARM3 to use the MESOPUFF-II dispersion parameters did not bring the modeled concentrations appreciably closer.

3.3.2 Meteorological Processor Comparisons

Since different options in the air quality models, which should force them to be nearly the same, could not account for the discrepancies in the concentrations calculated in the initial runs, the meteorological fields generated by the models' respective processors were examined. Each model treats the meteorological inputs somewhat differently. The MESOPUFF-II uses a two layer representation of the mesoscale winds. The lower layer (Level 1) is an average wind defined between the surface and the mixing depth, while the upper level wind (Level 2) is an average between the mixing depth and an arbitrarily defined upper bound, usually 700 mb. The ARM3 allows the selection of the number of layers to represent the winds. In the test cases run, pursuant to this discussion, six vertical layers were chosen. An average wind for each of these layers is calculated by the ARM3 meteorological processor. The methods used to generate the mixing heights in the two models are somewhat different. This will be discussed further below.

3.3.2.1 Wind Fields: The wind fields generated by the MESOPUFF-II processor are spatial and temporal interpolations of the surface and upper air observations. The method for calculating the mixed layer wind at each point follows (Scire *et al.*, 1984a):

(1) A representative rawinsonde sounding (00 or 12 GMT) is selected based upon the stability class at the nearest surface station to the grid point and the time of day. Neutral/unstable and stable conditions are assumed to be represented by the 00 GMT and 12 GMT sounding, respectively.
(2) Using the sounding selected in Step (1), vertically averaged u (easterly) and v (northerly) wind components are computed through the layer from the surface to the grid point mixing height.
(3) The ratio, R, of the layer-averaged wind speed to the surface wind speed at the rawinsonde station, and the angular difference in the wind direction, $\Delta\Theta$, between the layer averaged and surface winds are calculated.

(4) The hourly surface wind data are used to calculate spatially interpolated surface wind components (u_s,v_s) at each grid point. Data from all surface stations within a user-specified 'scan-radius' of a grid point are used to compute (u_s,v_s) according to

$$(u_s, v_s)_{ij} = \frac{\sum_k \frac{\alpha_s}{r_s^2} \bullet (u_k, v_k)}{\sum_k \frac{\alpha_s}{r_s^2}}$$

where:

u_s,v_s are the easterly and northerly components of the surface wind at grid point (i,j),

u_k,v_k are the easterly and northerly components of the surface wind at surface station k,

r_s is the distance from the surface station to grid point (i,j), and

α_s is an alignment weighting factor (α_s = 1-0.5 $|\sin \phi_s|$, where ϕ_s is the angle between the observed wind direction and the line from the surface station to the grid point).

For equal values of r_s, alignment weighting causes winds at a station directly upwind or downwind of a grid point to be weighted twice as heavily as the winds for a station at right angles to the grid point.

(5) The mixed layer averaged wind at the grid point is calculated by multiplying the surface wind speed at the grid point from Step (4) by the wind speed ratio, R, at the nearest rawinsonde site. Similarly, the surface wind direction is adjusted by the wind direction factor, $\Delta\Theta$.

Vertically averaged winds from the mixing height to the 850 mb, 700 mb, or 500 mb levels are computed in the following manner. The 00 GMT and 12 GMT winds at each rawinsonde station are first interpolated in time, and then vertically averaged through the layer from the grid point mixing height to the selected level (e.g., 700 mb). The winds at grid point (i,j) are obtained from the previous equation, with the summation over rawinsonde stations instead of surface stations. Only rawinsonde stations within a 'scan-radius' of the grid point are considered.

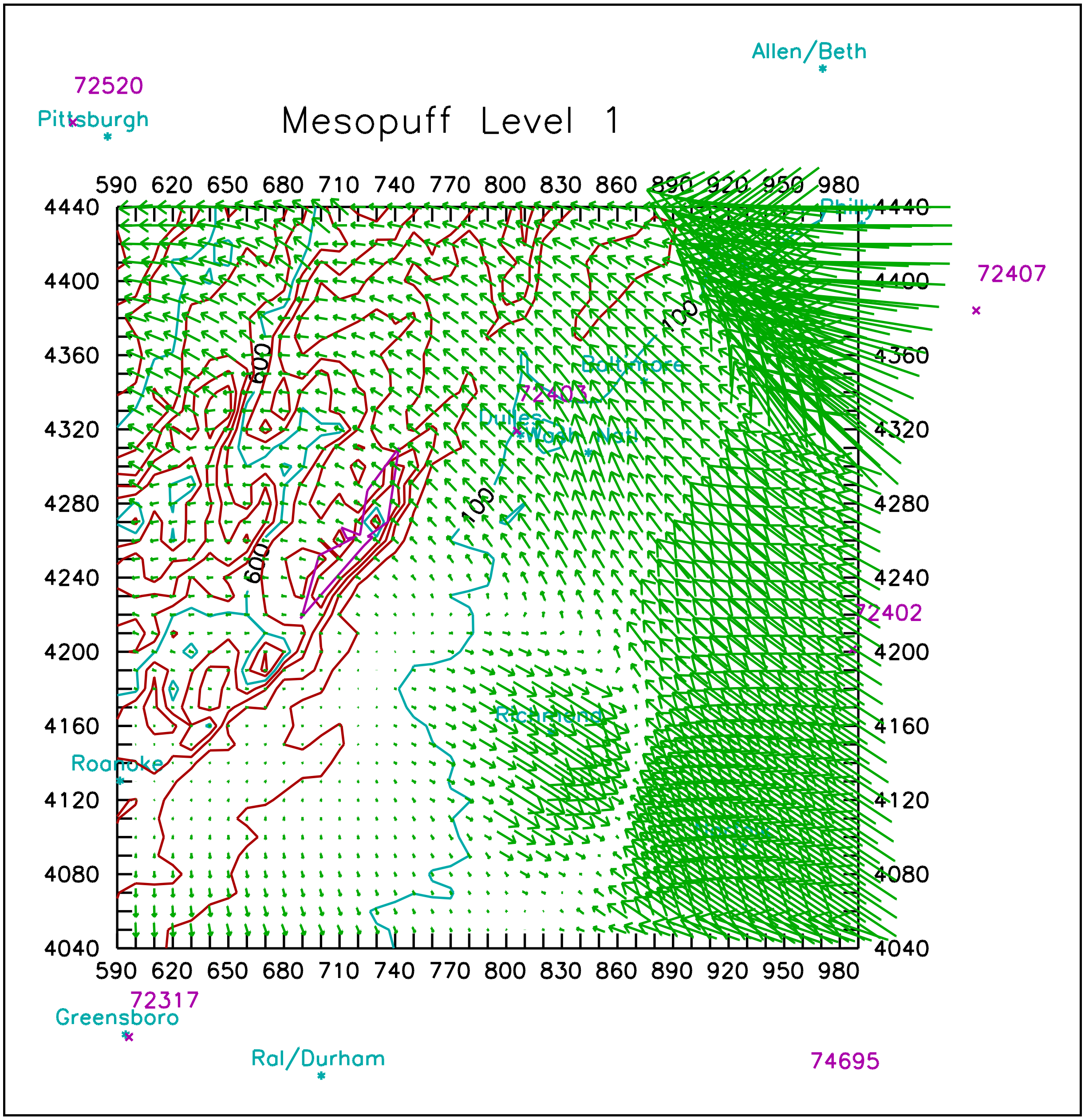

Figure 2a - Wind Vector Plot for July 21, 1984, 1200 LST. Level 1 winds are the layer average between the surface and the mixing depth.

Figures 2a and 2b are examples of the wind fields generated by the MESOPUFF processor for July 21, 1984 at 1200 LST. The effects of the 'scan-radius' and the influence of a deviant surface station on the calculation of mixed layer average (Level 1) winds can be seen in the vicinity of Richmond. There are also some aberrant winds generated in the vicinity of

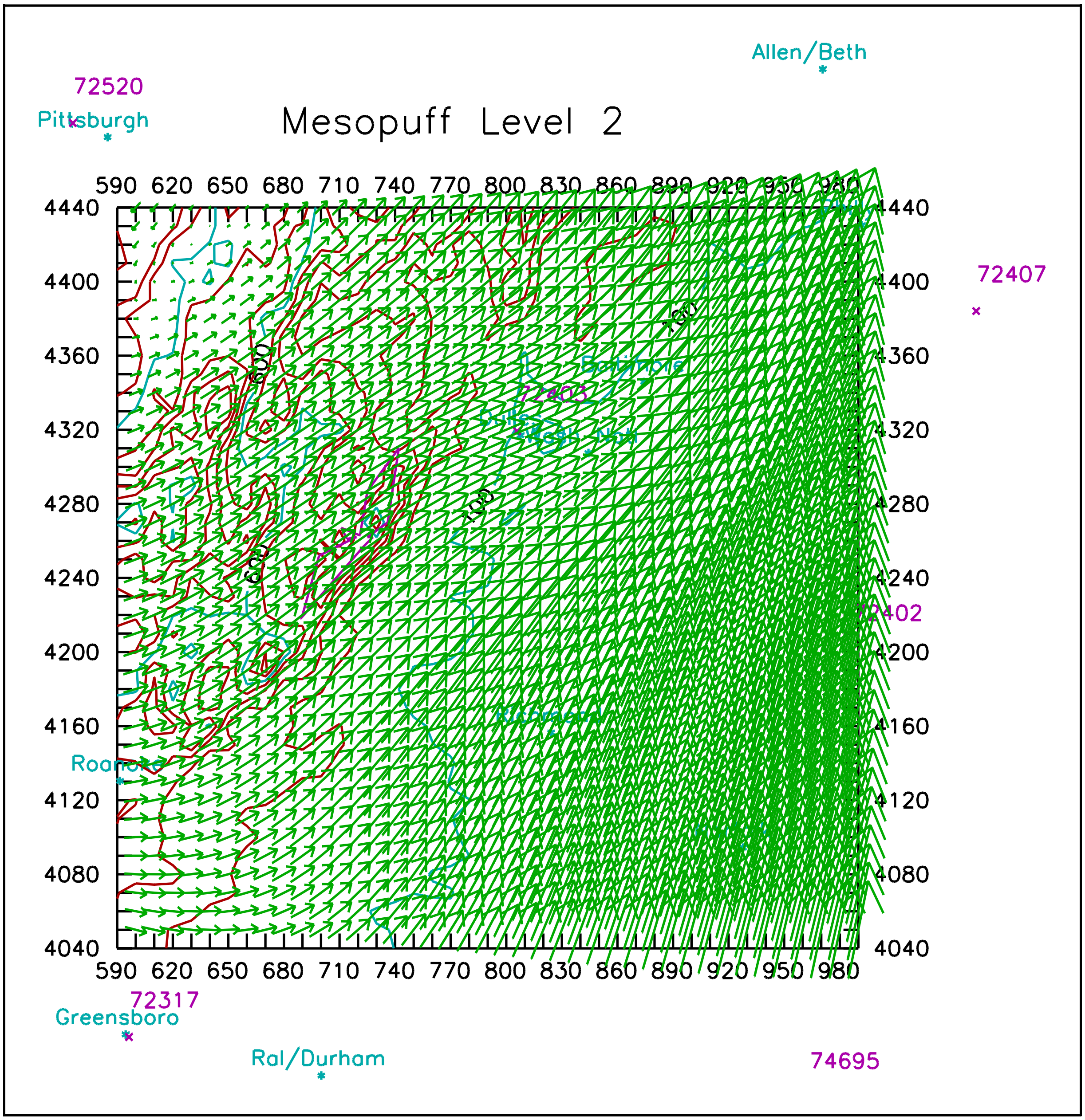

Figure 2b - Wind Vector Plot for July 21, 1984, 1200 LST. Level 2 winds are between the mixing depth and 700 mb.

Philadelphia. It appears, however, that the model is generating a sea breeze along the coastal areas. The Level 2 winds are generally fairly smooth and uniform.

The ARM3 takes a somewhat different approach to calculating the wind field for the region of interest. The ARM3 meteorological processor was designed to account for the influence of terrain on the wind fields over a data sparse area. The ARM3 processor computes a three dimensional wind field. The ARM3 air quality model can use the vertical velocities, generated by the meteorological processor, to transport puffs. However, vertical velocities generated by diagnostic wind models over complex terrain are highly suspect and are not recommended for use in the air quality model. Therefore, the remaining discussion will only pertain to the formulation of the horizontal components of the wind, although some of the procedures for calculating the vertical component can influence the calculation of the horizontal components.

The ARM3 processor uses "domain mean" parameters to initialize the entire modeling domain, then computes the effects of terrain on that flow and finally incorporates the observations into the terrain modified flow in the vicinity of the observations. The rationale for this is the supposition that the domain mean winds, modified for the terrain effects, better represent the flow in data sparse areas than relatively distant observations. In the ARM3 processor, the domain mean wind is defined from the sounding at the "central-most" station. The domain mean horizontal flow is modified to account for the effects of slope flows and blocking effects. The observations are incorporated into the modified mean flow through a user-specified weighting factor, such that grid cells near an observation give the observation relatively greater weight and cells more distant from any observations are weighted more heavily toward the modified mean flow.

A slope flow vector is calculated for each grid cell and added to the gridded domain mean (i.e., horizontally uniform) wind field. The slope flow parameterization does not account for any nonlinear interaction of slope flow with ambient flow. For any slope angle, α, the speed, S, of the parameterized slope flow is defined as:

$$S = S_0\left(\frac{dT}{dz}\right) \bullet f_1(t) \bullet f_2(\alpha)$$

$$\text{where:}\begin{cases} S_0\left(\frac{dT}{dz}\right) = \textit{The slope flow amplitude based on the domain-scale temperature lapse rate} \\ f_1(t) = \pm 1 \textit{ depending on the time of day } (-1 \textit{ for downslope}, +1 \textit{ for upslope}) \\ f_2(\alpha) = \textit{variability of the slope speed with slope angle} \end{cases}$$

Blocking effects are calculated from the gridded horizontal wind field, the available atmospheric stability information, and the gridded terrain heights. A local Froude number is calculated at each grid point. The Froude number is defined as:

$$F_r = \frac{S}{(N\Delta h)}$$

$$\text{where:}\begin{cases} S = \textit{the grid-point wind speed} \\ N = \textit{the Brunt-Vaisala frequency, defined as:} \\ \quad \sqrt{\left(\frac{g}{\theta}\right)\left(\frac{d\theta}{dz}\right)} \quad \textit{where } g = \textit{acceleration of gravity} \;\&\; \theta = \textit{potential temperature} \\ \Delta h = \textit{the effective terrain height at the grid-point} \end{cases}$$

If F_r is less than a critical Froude number, F_{rc}, usually equal to 1, and the horizontal wind at a given grid point has an uphill component, the horizontal wind is adjusted so that flow is in a terrain-tangent direction with no change in speed. If F_r is greater than F_{rc}, then flow is not adjusted.

After the domain mean flow is adjusted for both the kinematic effects of terrain and thermodynamic blocking effects, the available observational data are combined with this field to produce a final gridded wind field. This involves interpolation, smoothing of the analyzed field, computation of a vertical velocity field and a minimization of the three-dimensional divergence. The discussion here will only focus on the interpolation of the observational data into the modified domain mean wind field, since this feature will most affect future considerations of the ARM3 wind fields.

The procedure for interpolating both the surface and upper air data is a modified inverse weighting scheme. The interpolation is carried out separately for each model level. Unless otherwise specified, all surface wind observations are incorporated into the lowest model level. Upper-air observations are first vertically and temporally interpolated to model levels and desired simulation times. The terrain adjusted, domain mean horizontal components of the wind at each grid point, $(u,v)_1$, are modified to yield the observationally interpolated wind, $(u,v)'$ as follows:

$$(u,v)' = \frac{\sum_k \left[r_k^{-n} (u_0, v_0)_k \right] + R_1^{-n} (u,v)_1}{\sum_k r_k^{-n} + R_1^{-n}}$$

where:
- r_k = horizontal distance station k to grid-point
- R_1 = weighting factor for the diagnostic wind field
- n controls the relative influence of the observations
- $(u_0, v_0)_k$ = the observed wind at station k

This procedure weights the step 1 wind field, $(u,v)_1$, heavily in regions far removed from observations. The degree of influence exerted by the step 1 wind field is inversely related to the value of parameter R_1. The exponent, n, controls the relative influence of observations distant from a given grid point.

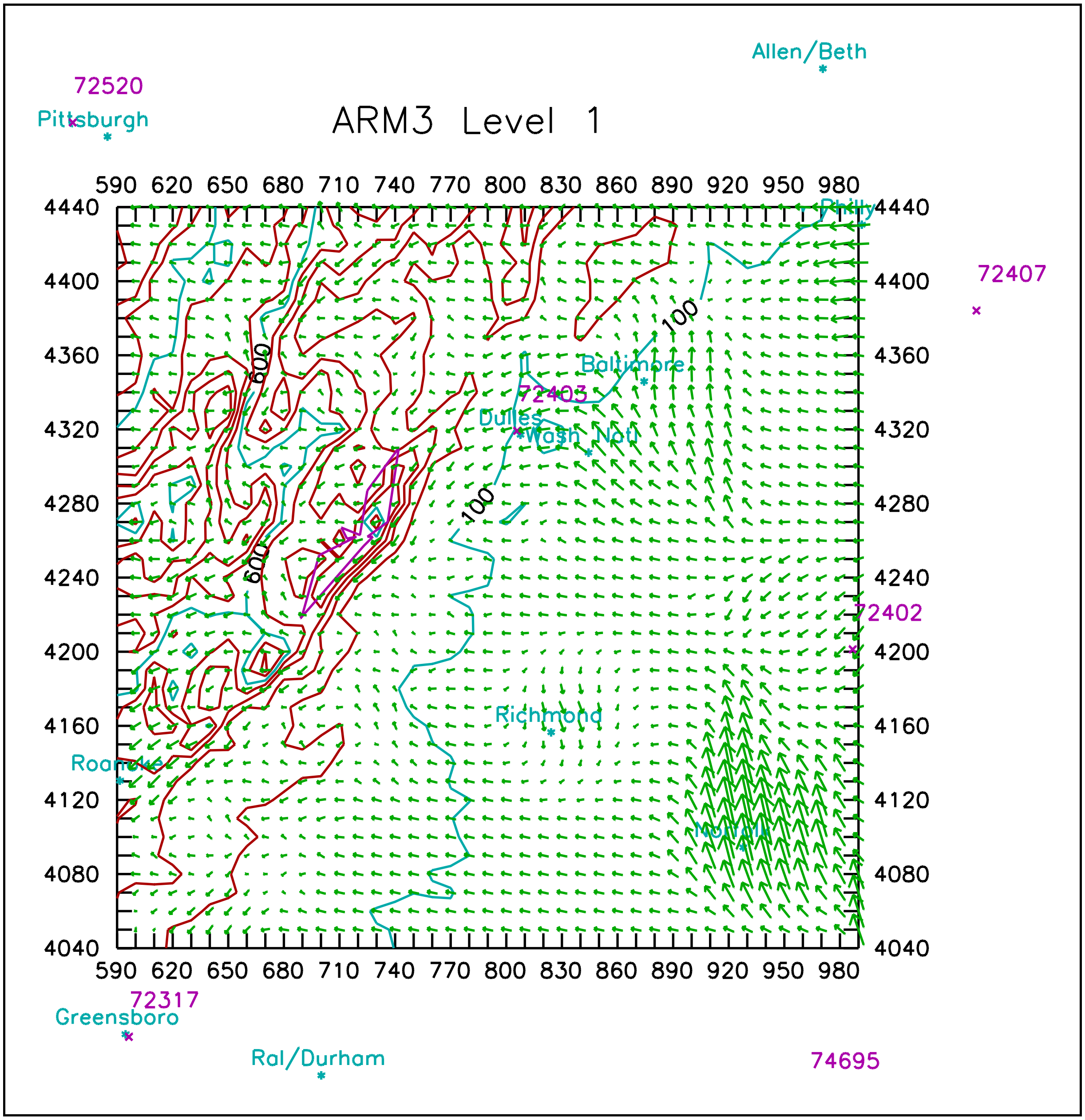

Figure 3a - ARM3 wind field for level 1, 10 meters, for July 21, 1984.

The wind fields generated by the ARM3 meteorological

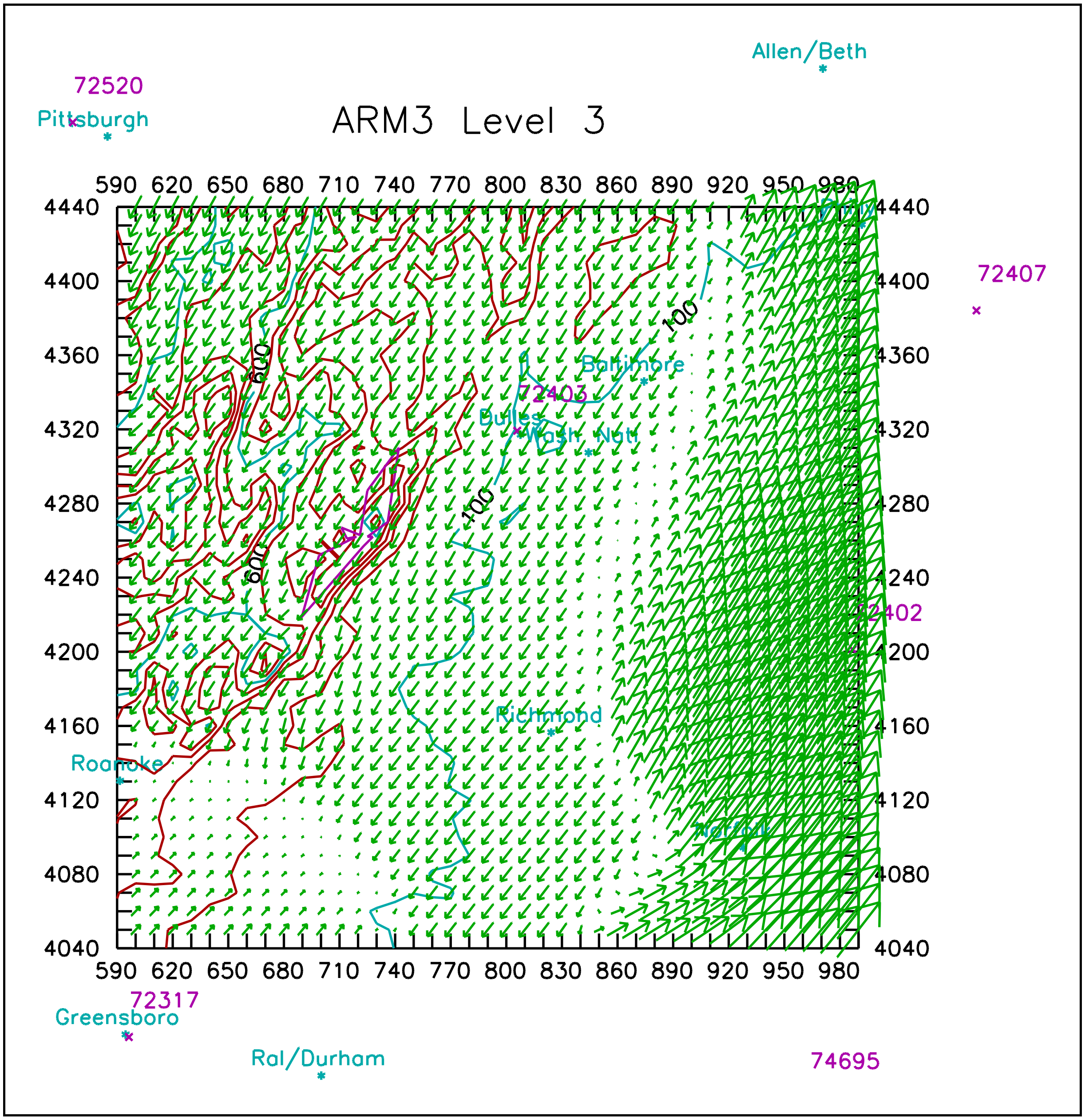

Figure 3b - ARM3 wind field for level 3, 300 meters, for July 21, 1984.

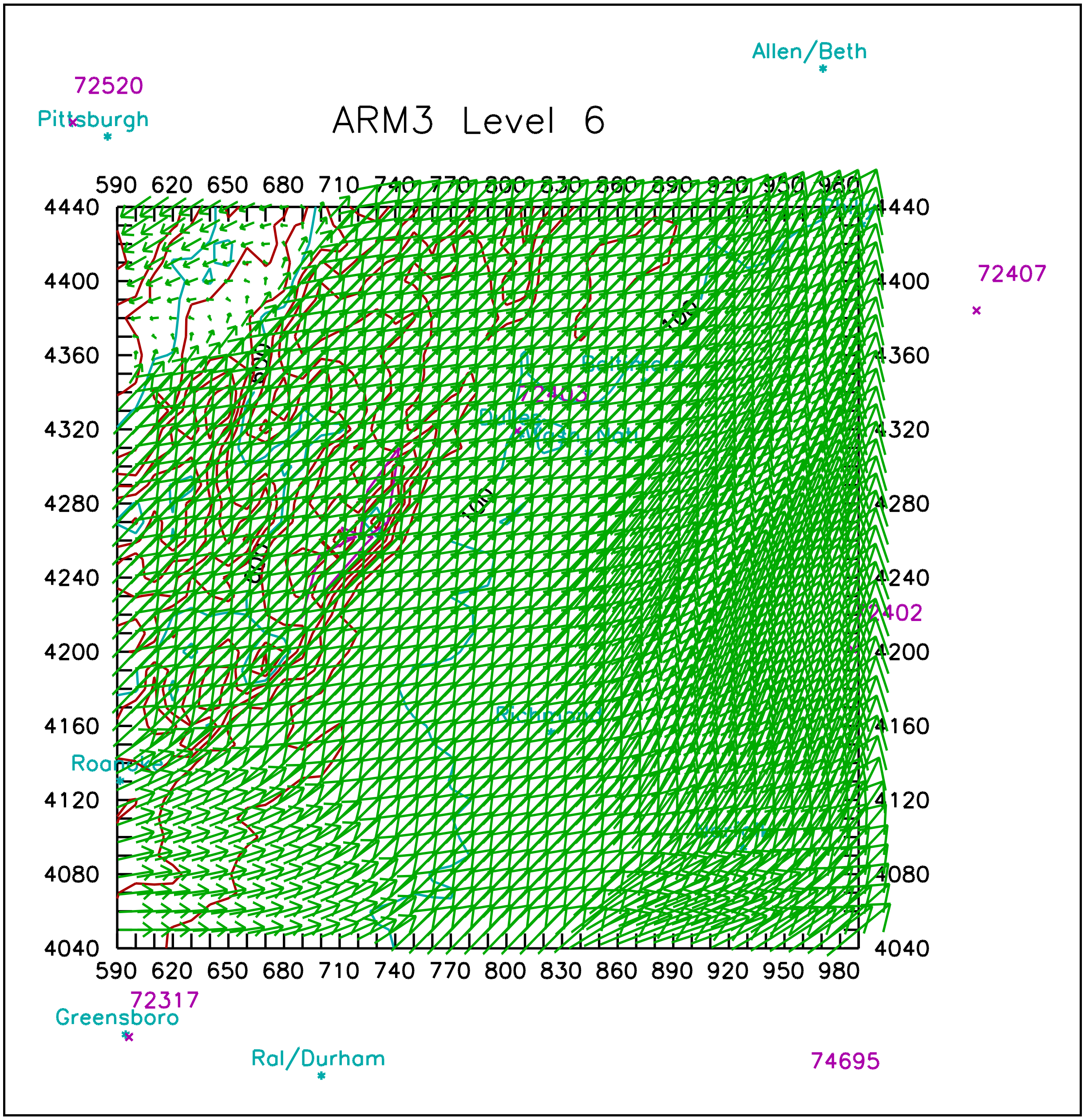

Figure 3c - ARM3 wind field for level 6, 2400 meters, for July 21, 1984.

processor for July 21, 1984, at 1200 LST (Figures 3a, 3b, and 3c) exhibit markedly different features than those generated by the MESOPUFF-II processor. First, it must be noted that the MESOPUFF-II winds are mixed layer averaged winds, whereas the ARM3 generated winds represent thinner layers of fixed thickness, above ground level. Although the vector fields of

Figure 2 represent somewhat different layers than those in Figure 3, some similarities might be expected. First the 10 meter field of Level 1 exhibits a relatively slow flow field. The influence of the interpolation scheme around surface stations is quite evident, particularly in the vicinity of Richmond, where the vectors are at about 90° from the mean flow around Richmond. Other than some of the local station influences, there is little resemblance between the ARM3 and MESOPUFF-II Level 1 wind fields. The 300 meter winds generated by the ARM3 meteorological processor (Figure 3b) might be expected to be more similar to the MESOPUFF-II Level 1 field (Figure 2a), since it represents a mixed layer average and since the ARM3 300 meter winds should be relatively representative of the mixed layer around 1200 LST; they are, however, quite disparate. Also, 300 meters might be the expected plume height of a relatively large source with a moderately tall stack. The MESOPUFF-II winds reach speeds of 18.9 m/s in the northeast corner of the domain. The ARM3 generated winds only reach 9.4 m/s. Both models have an area of stronger winds along the coastal area, but the wind directions are shifted by approximately 90°. The inland winds of the ARM3 Level 3 are relatively uniform from the NE (see Figure 3b), with the exception of the southwest corner of the modeling domain where they are light from the SW. The MESOPUFF-II winds are much more variable. Again the wind directions are shifted by about 90°. The MESOPUFF-II winds above the mixed layer and the ARM3 2400 meter winds are very similar. The wind directions are about the same and the overall magnitude of the winds is about the same.

As previously noted, the two models handle the generation of winds above the surface somewhat differently. The MESOPUFF-II approach uses the deviation between the surface and upper air wind speeds and directions at the time of the soundings and the current hour's surface data to calculate the wind speeds and directions within the surface layer. Whereas, the method used by the ARM3, above the first layer, is to use spatially and temporally interpolated upper air data to perform its calculations. Furthermore, the ARM3 interpolations of data are not performed until after a uniform "first guess" wind field is modified for the effects of terrain and the modified first guess field is given higher priority in the interpolations in areas more removed from observations. Therefore, the general directional features of the flow fields between the respective models' lowest levels are similar, since both make use of the surface station data. However, with the six layer representation of the atmosphere used in ARM3, the winds at levels above the first level, and below the height of the mixing depth, are quite different than those calculated by MESOPUFF-II. The method for calculating winds above the mixed layer, however, is similar between the two models in that both use only spatially and temporally interpolated winds for their respective calculations. The ARM3 still uses the modified first guess field, but at higher levels there is generally much more uniformity to the overall flow field.

3.3.2.2 Mixing Height: Mixing heights are another parameter which could potentially result in dramatically different concentrations calculated by the two air quality models. MESOPUFF-II and the ARM3 both calculate a mechanical mixing depth for the nighttime hours and a mechanical and convective mixing height during the daytime and use the greater of the two as the mixing depth. The two models use similar, but somewhat different, algorithms to calculate the mixing depth, which yields different results.

The convective mixing depth algorithm in the MESOPUFF-II meteorological processor assumes that during daylight hours, solar radiation reaching the ground produces an upward flux of sensible heat and the development of a well-mixed adiabatic layer. If the hourly sensible heat, H, is known, the mixed height z_i at time t+1 can be estimated from time t in a stepwise manner.

$$(z_i)_{t+1} = \left[(z_i)_t^2 + \frac{2H(1+E)\Delta t}{\psi_1 \rho c_p} - \frac{2(\Delta\theta)_t (z_i)_t}{\psi_1} \right]^{\frac{1}{2}} + \frac{(\Delta\theta)_{t+1}}{\psi_1}$$

$$(\Delta\theta)_{t+1} = \left(\frac{2\psi_1 E H \Delta t}{\rho c_p} \right)^{\frac{1}{2}}$$

where:
- ψ_1 = *the potential temperature lapse rate in the layer above* z_i
- Δt = *the time step* (3600 *s*)
- E = *a constant* (~0.15)
- $\Delta\theta$ = *the temperature discontinuity at the top of the mixed layer*

The sounding at the nearest rawinsonde station to the grid cell is used to determine the lapse rate ψ_1.

The daytime mechanical mixing depth is calculated from:

$$z_i = \frac{B u_*}{(f N_B)^{\frac{1}{2}}}$$

where:
- f = *the Coriolis parameter*
- B = *a constant* ($\sqrt{2}$)
- u_* = *the friction velocity*
- N_B = *the Brunt-Vaisala frequency in the stable layer aloft*

The nighttime mechanical mixed layer is determined from:

$$z_i = 2400 u_*^{\frac{3}{2}}$$

Examples of a daytime and nighttime MESOPUFF-II generated mixing depth field are shown in Figures 4a and 4b. The daytime mixing depths generated by MESOPUFF-II exhibit some extreme discontinuities from one grid cell to the next. This is a result of using only the nearest rawinsonde station sounding to calculate the convective mixing depth, rather than an interpolated field. The nighttime mixing depths make a much smoother transition from one cell to the next. The daytime mixed depth values range from 552 meters to 1759 meters, whereas the nighttime mixed depth values range from 10 meters to 1360 meters.

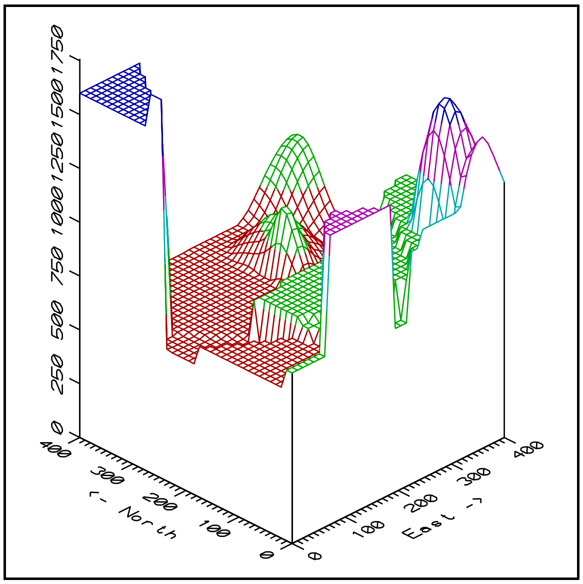

Figure 4a - MESOPUFF-II Mixing Heights for July 21, 1984, 1200 LST

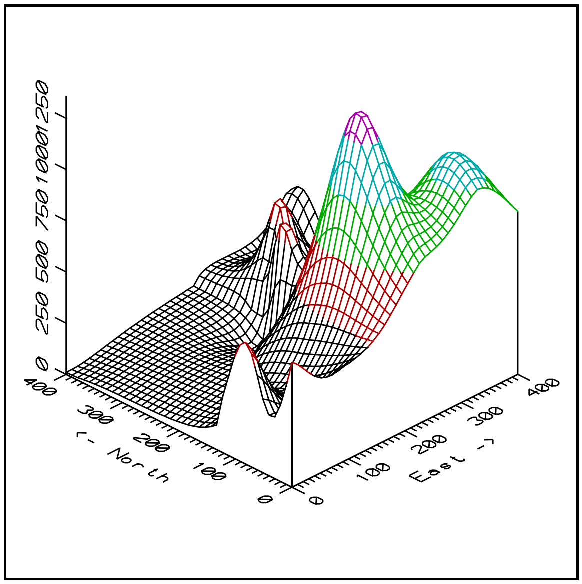

Figure 4b - MESOPUFF-II Mixing Heights for July 21, 1984, 0000 LST

In the ARM3 system, the daytime convective mixed depths are determined as the height of the intersection of the hourly surface potential temperature and the morning potential temperature sounding. Cold or warm air advection is accounted for by adjusting the hourly surface potential temperature values according to an advection rate. The advection rate is determined from the difference in potential temperature between the afternoon and morning sounding at a height above the convective mixing height.

The ARM3 mechanical mixing depth is the same for both daytime and nighttime conditions.

$$H_{mech} = 53U_{Free\ Stream}$$

where: $U_{Free\ Stream}$ *is taken to be the wind speed at* 3000 *meters*

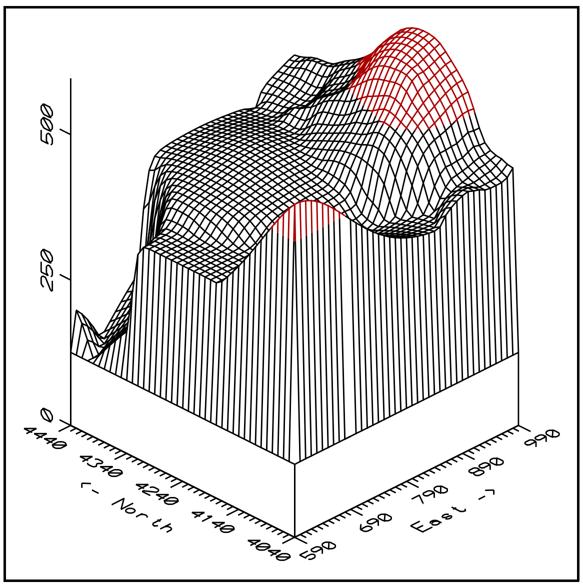

Figure 5a - ARM3 Mixing Heights for July 21, 1984 1200 LST.

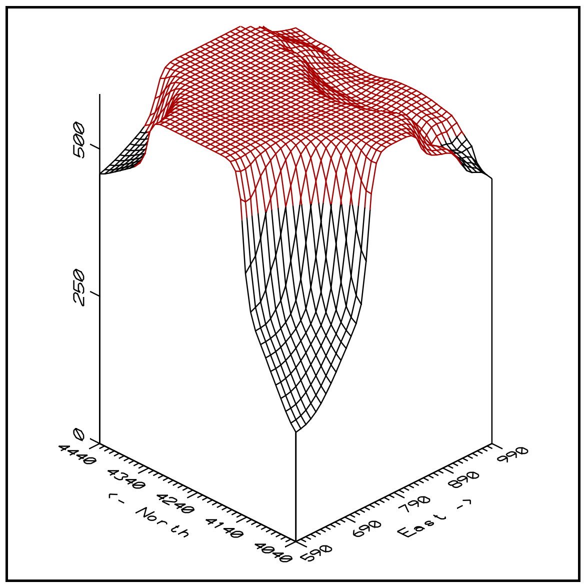

Figure 5b - ARM3 Mixing Heights for July 21, 1984 0000 LST.

The ARM3 generated fields (Figures 5a and 5b) show relatively smooth fields for both daytime and nighttime. The actual heights, however, are much lower during the daytime than those calculated for MESOPUFF-II, ranging from 125 meters to 596 meters. During the nighttime, the values range from 185 to 593. So while the ARM3 mixing height fields do not exhibit the discontinuities from one cell to the next that the MESOPUFF-II daytime fields show, they do not show any appreciable diurnal variation.

To further illustrate this, domain average mixing heights were calculated for each model and plotted (Figure 6). The

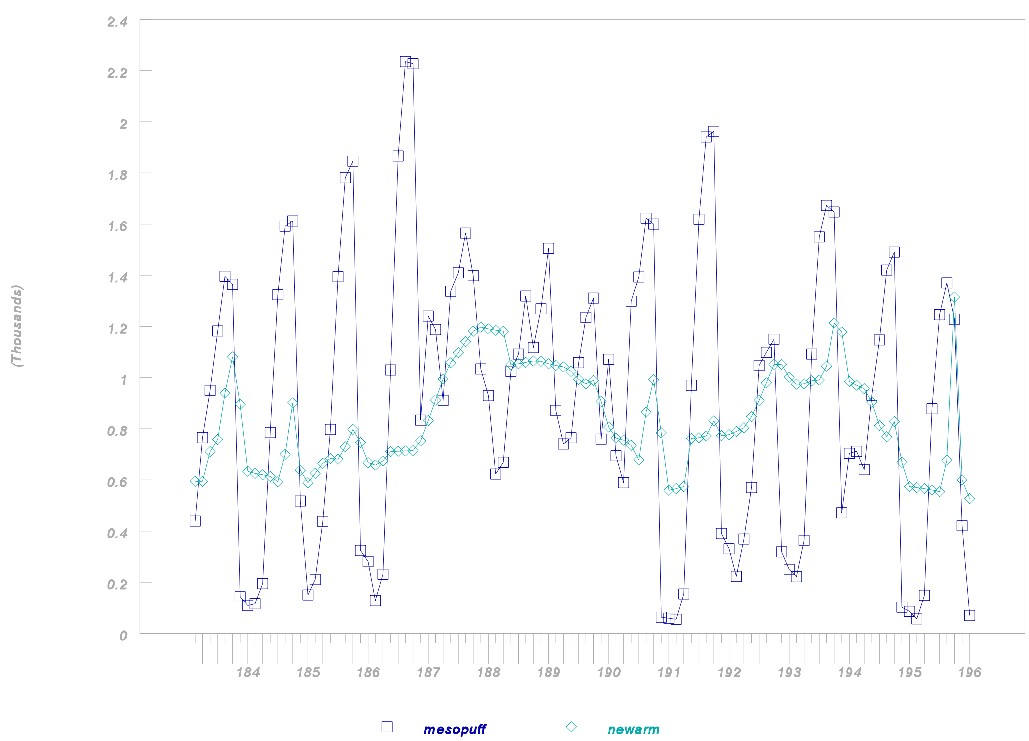

Figure 6 - Plot of hourly average mixing depths (m), plotted every third hour.

MESOPUFF-II heights show diurnal variation over the entire time-span plotted, while the ARM3 mixing heights show almost no relationship to the diurnal cycle. This can be partially explained by the method used to calculate the mechanical mixing depth. The choice of the 3000 meter wind speed as an indicator of the free stream wind will almost always force the wind to be at least on the order of 5 m/s. If the term U in the ARM3 mechanical mixing equation is set to 5, then the minimum mixing depths will generally be on the order of 265. In order for reasonable nighttime mixing heights to be calculated, the 3000 meter wind would have to be more on the order of 1 m/s. At that altitude, however, a wind speed of 1 m/s is not likely to occur very often. The daytime mixing depth calculations, generated by the ARM3, are generally too low. The reason for this has not been investigated at this time.

3.3.2.3 Meteorological Field Discussion: The wind fields generated by the two models are each based on distinctly different approaches to interpolating surface and upper air observations. Both methods have some significant problems. For the stated purpose of IWAQM, the MESOPUFF-II approach lacks the ability to treat the effects terrain will have on the mean flow, except as much as local observations represent the mean flow in the terrain. The mixed depth average wind speed and direction used by MESOPUFF-II can be both a strength and a weakness. The strength of the system is that it provides some other information to the interpolation scheme between 12 hour soundings by using the relationship between the surface and upper air data at the time of the twelve hour soundings. One problem with this, however, is that it is based upon the assumption that the surface and upper air data are indeed coupled. It is quite possible that under some circumstances, particularly in complex terrain, that the surface and upper air winds are independent from each other. Hence, the use of the relationship between the surface and upper air winds may yield spurious results. Another factor to consider with respect to the mixed depth average winds is the behavior of the mixed depth, as illustrated in Figures 4a and 4b. In the northwest corner of the 1200 LST MESOPUFF-II mixing height field (Figure 4a), the mixing depth jumps from a height of around 500 meters to approximately 1600 meters in adjoining grid cells. Thus, the mixed layer average wind will represent very different quantities between those adjoining cells.

The ARM3 wind fields ostensibly meet the IWAQM criteria of accounting for the effects of terrain on the wind fields. The method the ARM3 uses to account for terrain effects warrants some discussion. The wind field generating portion of the model is called the Diagnostic Wind Model (DWM). The order of analysis that the DWM uses is to first generate a horizontally uniform "first-guess wind field." This first-guess field is defined from the central-most sounding found in the modeling domain. The effects of terrain, blocking and kinematic effects, are applied to this first-guess, mean flow field. The remaining surface and upper air observations are then applied with the weighted interpolation scheme described earlier. The strength of this approach is that it can yield a more reasonable flow field in complex terrain where meteorological observations are sparse. It does, however, introduce some problems when generating a regional scale flow field.

If a wind field is to be generated over a relatively small air basin, which includes complex terrain, where one may have only one sounding within the domain, the aforementioned use of a first-guess wind field is probably valid. When one is generating a wind field over a larger domain, however, the assumption of a first guess-field, based on one sounding, is probably not appropriate. If, for example, a major topographic barrier runs through the domain, it is quite likely that the air flow on the opposite sides of the barrier may be very different. Blocking, for example, will only occur on the windward side of the barrier. If only one sounding is used, this blocking and subsequent turning of the wind will only occur on one side of the barrier, where in reality there may be upslope flows on both sides of the barrier, with subsequent terrain modifications to the flow. Thus, while one of the strengths of the ARM3 wind generation model is its ability to treat flows in complex terrain, its implementation may ultimately lead to the generation of spurious winds on the sides of barriers opposite the station used to generate the first-guess field.

The generation of mixing depths by the two models is dismal. The implementation of the MESOPUFF-II algorithms yields large discontinuities in adjoining grid cells, while the ARM3 implementation of the calculation of mixing depths did not reproduce any expected diurnal variability. As noted earlier, the reasons for the behavior of the two algorithms are generally understood. The MESOPUFF-II algorithms only rely upon data from the nearest sounding. There has been no attempt to use a weighted interpolation between soundings. Therefore, if adjoining grid cells are nearer to different soundings, the calculated mixing depths may be quite different. The only independent variable in the ARM3 mechanical mixing depth calculations is the 3000 meter wind speed at that grid cell. At an altitude of 3000 meters, the wind speed will generally be relatively high, thus leading to spuriously high mixing depths at night. The daytime mixing depth calculations, generated by the ARM3, are too low. The reasons for this have not been investigated at this time; methods which overcome the problems with both modeling systems' mixing depth algorithms have been identified and should be implemented in Phase 2.

3.3.3 Further Air Quality Model Comparisons

After reviewing the mixing height fields and the wind fields, a likely possibility for the higher concentrations calculated by the ARM3 model was the tendency for the mixed layer height to stay at relatively low levels over extended periods. To test this hypothesis, the previously run test case was run with the MESOPUFF-II generated mixing depth fields and the ARM3 generated wind fields as input to the ARM3 air quality model. This resulted in little appreciable change in the calculated concentrations; the ARM3 maximum concentrations were still considerably higher than those generated by MESOPUFF-II. Similarly, when the MESOPUFF-II air quality model was run using the mixing depths generated by the ARM3 meteorological processor, the calculated maximum concentrations did not change appreciably.

The wind field from the MESOPUFF-II model was substituted as input to the ARM3 air quality model. This produced concentrations quite similar to the MESOPUFF-II air quality model, using the same wind field. Since this change in the wind fields generated such different results, it was anticipated that there might be a region of very light winds generated by the ARM3 processor. Examination of the plots of the gridded wind fields of the two models for the time preceding the maximum concentration calculation, did not elicit any obvious reason for the vastly different concentration calculations. The examinations focussed on the Level 2 and 3 fields from ARM3 and the Level 1 field from MESOPUFF-II, since these were expected to be the respective transport levels for the hypothetical source being modeled in the test cases. To check which levels were being selected by the ARM3 to transport puffs, the code was examined. This lead to the discovery of a fundamental coding error.

The ARM3 calculates the center of mass of a puff and uses the wind level at the altitude of the center of mass to transport the puff. A subroutine is called to extract the wind data for the appropriate grid cell and level. The algorithm defined the transport altitude as a fraction of the total model domain height. This fraction was then compared against the absolute magnitude of the height of the various wind levels to select the level of the wind to use. This resulted in a normalized transport altitude, which would always be less than or equal to 1, being compared with an array of heights ranging from 10 to 2400 meters. Thus, the model would always choose the 10 meter wind level for all of its calculations. The 10 meter winds did exhibit some very light, almost calm conditions between the hypothetical source and the receptor area in the test case. Since the model was always selecting the 10 meter winds, when the MESOPUFF-II mixed layer average winds were substituted into appropriate levels in the ARM3 input files, the ARM3 would always be picking the MESOPUFF-II mixed layer winds as its 10 meter winds and thus was yielding similar results.

Subsequent to the discovery of the coding error, the code was patched, and the ARM3 meteorological and air quality modeling system was again run. The concentrations from this run were of the same order as those calculated by the MESOPUFF-II.

3.3.3.1 Model Comparison Discussion: Until a more refined technique can be evaluated, neither of the models under consideration by the IWAQM to use in the interim are totally satisfactory. With respect to the meteorological processors, the MESOPUFF-II processor should incorporate a weighted interpolation algorithm in the calculation of mixing depths to avoid the extreme gradients encountered in the current formulation. The ARM3 processor, on the other hand, should employ different algorithms for calculating mixing depths and should change the order of analysis in the diagnostic wind field calculations to start out with a field interpolated from the observations as the first-guess field, upon which the kinematic and blocking effects of terrain should be applied.

The MESOPUFF-II model does not explicitly include any treatment for the effects of terrain on long range transport and dispersion. This is a relatively major deficiency with respect to the needs of the IWAQM. While the ARM3 incorporates algorithms to treat such effects, the model has been found to have a number of coding errors which render its use suspect.

One of the rationales for limiting the interim modeling choices to either the MESOPUFF-II or the ARM3 was their performance relative to other similar models. After the coding error, described above, was discovered in the current version of the ARM3 code, an examination was made of the originally released version of the code. The code was found to contain the same fundamental error found in the current version. Thus, the evaluations of the ARM3 were carried out using only the surface wind fields. For the case of the Oklahoma data, this is not necessarily a major problem, since it was based on a surface tracer release. However, the Savannah River evaluation involved an elevated release into a wind level above the surface level. If the surface level and the upper level were very similar, the ARM3 evaluation results may be valid, but unless the corrected model is re-run with the Savannah River data, confidence should not be placed in the Savannah River comparisons.

4. REGULATORY CONSIDERATIONS FOR THE USE OF LONG RANGE TRANSPORT MODELS

The *Guideline* explicitly identifies certain steady-state, Gaussian plume models which are preferred for calculating concentrations of inert pollutants for source-receptor distances of less than 50 km. The MESOPUFF-II model has been shown to replicate steady-state, Gaussian plume results, under many conditions, when it is run with steady-state meteorology and Pasquill-Gifford dispersion coefficients (Scire *et al.*, 1984a). When MESOPUFF-II is run in an operational mode, however, the results could be quite different, since the meteorology will be time varying and the simulated pollutant transport can be quite different than the steady-state approximation. Having two acceptable techniques (i.e., MESOPUFF II and a *Guideline* model) which can give different results for the same application is untenable for regulatory purposes. Therefore, while it would be desirable to run only one model, it will be necessary to run both a preferred, *Guideline* model and the recommended long range transport model for many permitting situations.

For estimating impacts on AQRVs, the approach need not be as operationally complicated. Since all AQRV analyses, covered by this recommendation, involve secondary pollutants, the use of MESOPUFF-II for all distance ranges was felt to be acceptable. Although the use of MESOPUFF-II for sources located close to the Class I area is questionable, their impact should be quite small due to the small travel times involved. Also, based on the very stringent Class I increments, any sources locating close to a Class I area will usually be unable to emit large quantities of primary pollutants.

Similarly, there are likely to be occasions when long range transport is to be considered, when it would be desirable to run a simpler model, for screening purposes, than the recommended long range transport model. In past applications, steady-state, Gaussian plume models have been used. Comparison runs of the MESOPUFF-II, run in a steady-state mode, and the ISCST2 model indicate that the ISCST2 will frequently produce similar or higher concentrations, but not under all circumstances. Since the MESOPUFF-II will use a spatially and temporally varying wind field when run in an operational mode, the concentrations it produces will generally be lower than those produced by the ISCST2 model. If, however, there are prolonged periods of near stagnation conditions or if recirculations occur, the ISCST2 will not necessarily produce conservative concentrations.

5. INTERIM RECOMMENDATIONS

From the review of the ARM3 and MESOPUFF-II models, the IWAQM found neither model to be totally satisfactory. However, due to the immediate need for a modeling system to estimate impacts from sources farther than 50 km from a receptor and to estimate the impacts on visibility and other AQRVs from all distances, the IWAQM is recommending that the MESOPUFF-II model be used for these analyses. This recommendation is to be considered interim, until a more suitable technique can be developed and tested. The IWAQM is recommending that MESOPUFF-II be run in a somewhat different mode than was previously suggested by EPA (EPA, 1988), and is recommending some approaches to integrating the long range modeling system with regulatory modeling requirements. A relatively simple method, using steady-state, Gaussian plume models, is suggested as a way to provide a first estimate of concentrations from long range transport. The recommendations herein are the suggestions of the IWAQM; implementation of these recommendations is a matter for the appropriate regulatory agencies and should be done in consultation with the appropriate EPA regional office.

The following recommendations are divided into two categories. The first is referred to as a "Level I" analysis. This relatively simple analysis is expected to provide a conservative estimate of concentrations due to long range transport. If the Level I estimates indicate that adverse conditions may be caused in the Class I area of concern, then a "Level II" analysis, using the MESOPUFF-II modeling system, should be undertaken.

5.1 Protocol for Level I Long Range Transport Analysis

The IWAQM is suggesting that a steady-state, Gaussian plume model may be acceptable as a first level long range transport analysis technique under many conditions. It is anticipated that this first level technique will, under most conditions, yield a conservative estimate of ambient air quality concentrations. However, under conditions of extended stagnation or where recirculation patterns or convergence zones are known to occur, this Level I technique should not be used. If a Level I analysis indicates that there are exceedances of the appropriate parameters, the more refined analyses, using the Level II long range transport models, should be run for all meteorological conditions, not just those identified through the Level I technique. Level I analyses will consist of running the appropriate steady-state, Gaussian plume models with five years of meteorological data. Steady-state Gaussian plume models used for Level I long range transport analyses should utilize bivariate plume dispersion factors. It is generally anticipated that plume impaction models, utilizing uniform horizontal plume dispersion, would not be appropriate for a long range transport analysis.

While the IWAQM is suggesting a relatively simple, Level I, technique, it should not be construed as an endorsement of that approach. With limited testing, the suggested Level I technique appears to yield higher ambient pollutant estimates than the Level II procedures. However, if there is any question about the technical veracity of using the Level I technique in a given situation, then it is completely appropriate to proceed directly to a Level II analysis.

In general, the steady-state Gaussian plume models will yield a high estimate of concentrations at distances beyond 50 kilometers, due to the spatially varying paths of puffs in the recommended long range transport model. As mentioned previously, this is not always the case. Therefore, it is expected that application of the Level I techniques will need to be reviewed by those with sound professional judgement. Under light wind conditions or under recirculation conditions, the MESOPUFF-II model may yield higher concentrations than steady-state, Gaussian plume models. Therefore, if these conditions occur, the Level I analysis should be adequately assessed. These conditions are not necessarily generally defined; the IWAQM is not attempting to define them further. It is anticipated that as more experience is gained with the Level I and II techniques, further resolution on when either method is appropriate can be better elucidated.

Since many of Class I areas are located in complex terrain, the issue of the appropriate methods for applying Level I long range transport modeling techniques to these areas arises. Each analysis will have unique characteristics which must be evaluated on a case-by-case basis. In many cases, however, some of the following considerations will apply. As noted previously, models incorporating bivariate plume dispersion parameters are suggested for use in a Level I analysis. This suggestion is based on the presumption that after a plume has travelled 50 km or farther, it will have been affected by a variety of processes, land use, and terrain intervening along the trajectory of the plume. Therefore, it may not be appropriate to use a plume impaction model for these circumstances. Similarly, under many conditions, when long range transport is involved in moving pollutants to a Class I area, the plumes will be traversing steadily rising terrain. Under the constraints of existing, steady-state, Gaussian plume models, receptor heights are either restricted to be no greater than the height of the stack which emitted the pollutants, or in the case of some of the plume impaction models, the concentrations are considered to be zero if the elevation of the receptor is sufficiently far above the calculated plume height. Under conditions of steadily rising terrain, the air flow, and plumes imbedded in that flow, will tend to follow the terrain and become well mixed after a distance of 50 km. Therefore, the various simple terrain models, outlined in the *Guideline*, should generally provide a reasonable approximation of transport and dispersion under these conditions.

The results of the Level I technique will be analyzed somewhat differently for increment and NAAQS analyses than for visibility and other AQRV analyses. The methods for performing these first level long range transport analyses are discussed below.

5.1.1 Level I Long Range Transport Techniques for Analyzing Increment and NAAQS

If Level I methods are to be utilized for increment and NAAQS analysis, then all sources, whether closer or farther than 50 km should be analyzed assuming no conversion of SO_2 to $SO_4^=$ and NO_x to NO_3^- and no deposition. If that analysis indicates that the increments or NAAQS are being exceeded, then a full analysis, using the recommended long range transport model in combination with the steady-state Gaussian model, as described below, should be employed.

5.1.2 Level I Analysis Technique for Evaluating the Effects of Long Range Transport and Regional Visibility

If a Level I approach is desired, it should be assumed that all SO_2 has been converted to $SO_4^=$ and that all NO_x has been converted to NO_3^- in the analysis. Refer to Inset 1 for the appropriate method for converting SO_2 and NO_x to $SO_4^=$ and NO_3^-.

The procedures in Appendix B should be used to estimate the visibility impacts.

Calculation of $SO_4^{=}$ & NO_3^{-} For Visibility Screening

1. Run appropriate long range transport screening model.

2. Assume no conversion of SO_2 or NO_X to other species. (i.e. assume all NO_X is emitted as NO_2 and that all SO_2 remains inert at this step.)

3. Multiply the hourly concentrations of SO_2 and NO_X by the ratios of the molecular weights of the secondary species to the primary species.
   Note: The molecular weights of SO_2 and $SO_4^{=}$ are 64 and 96 and the molecular weights of NO_2 and NO_3^{-} are 46 and 62. Thus multiplying the concentration of SO_2 by 1.5 will yield the concentration of $SO_4^{=}$ and multiplying the concentration of NO_2 by 1.35 will yield the concentration of NO_3^{-}.

4. The averaging time of interest is generally 1-hour.

Inset 1 - Method for calculating concentrations of $SO_4^{=}$ and NO_3^{-} from SO_2 and NO_X.

5.1.3 Level I Analysis of Long Range Transport and Depositional Impacts

If a Level I approach is to be taken for depositional impacts, it should be assumed that concentrations of SO_2 and NO_X are deposited as SO_2 and HNO_3 (see Inset 2). Since the steady-state, Gaussian plume models do not actually remove any mass from the plume, when run in their recommended modes, this will provide a conservative deposition estimate.

Calculation of Deposition For Level I analysis

1. Run appropriate model for Level I analysis.

2. Assume no conversion of SO_2 or NO_X to other species. (i.e. assume all NO_X is emitted as NO_2 and that all SO_2 remains inert at this step.)

3. Multiply the concentrations of NO_X ($\mu g/m^3$), if applicable by the ratio of the molecular weights of the secondary species (HNO_3) to the primary species (NO_2).
   Note: The molecular weights of NO_2 and HNO_3 are 46 and 63. Thus multiplying the concentration of NO_2 ($\mu g/m^3$) by 1.37 will yield the concentration of HNO_3 ($\mu g/m^3$).

4. The majority of sulfur will be deposited as SO_2, so no conversion is necessary.

5. The averaging times for deposition will generally require a long term value (monthly, seasonal, or annual) and short term value (1, 3 or 24-hour). Since the Level I models will produce average values, they must be converted to total rates.

   Multiply the concentration of SO_2 or HNO_3 by the number of seconds in the averaging time of interest to obtain a total rate. (3.1536×10^7 seconds/year, 86400 seconds/day, 10800 seconds/3-hours, or 3600 seconds/hour)

6. Multiply the result of step 5 by the deposition velocity for the appropriate pollutant. (0.005 m/s for SO_2 or 0.05 m/s for HNO_3). This will result in a deposition value in units of $\mu g/m^2$.

7. To convert to kg/hectare, multiply the result of step 7 by 10^{-5}.

Inset 2 - Description of method to estimate deposition from SO_2 and NO_X concentrations.

5.2 Protocol for Level II Long Range Transport Analysis

The IWAQM is recommending that the MESOPUFF-II model be run for source-receptor distances of greater than 50 km, up to several hundred km, when predicting the concentrations for criteria pollutants. For impacts on AQRVs, the IWAQM is recommending the use of MESOPUFF-II for all source-receptor distances. It is also recommended that the analyst generally follow the recommendations in *A Modeling Protocol for Applying MESOPUFF-II to Long Range Transport Problems* (EPA, 1988); the primary exceptions to that protocol are the distance at which time dependent dispersion curves are used, the use of the chemical transformation and deposition algorithms (both wet and dry), and the use of five years of meteorological data. The IWAQM recommendations for model options and input parameters can be found in Appendix A.

The two areas where the previous protocol and the IWAQM protocol diverge are in the specification of the distance where time dependent dispersion curves are used to calculate puff dispersion and the use of the chemical transformation and deposition options. The previously suggested protocol for the use of MESOPUFF-II (EPA, 1992) stated that the distance at which the time dependent dispersion curves should be use was beyond 100 km. It was indicated that the reason for this choice was that the 100 km distance was used during the performance evaluations (EPA, 1986), which identified MESOPUFF-II as one of the better performing models. The reference to 100 km appears to have been erroneous. A summary article, describing the performance evaluations (Carhart *et al.*, 1989) stated:

> The Turner curves were established from experiments carried out over distances of 0-1 km from the source, and yet some models use the curves out to 100 km. In the MESOPUFF-II model, the transition from the Turner to the Heffter formulation is made at **10 km** from the

source (a recommended user-input value adopted in this study). On the other extreme are MESOPUFF and MESOPLUME, which specify 100 km as the transition distance.

Therefore, it seems clear that the performance evaluations were indeed carried out with the transition between distance and time dependent formulations set at 10 km. Thus the IWAQM is recommending that the model be run with the 10 km setting.

The previous protocol also recommended that the model be run assuming no chemical conversion or deposition of pollutants (either wet or dry). For the purposes of IWAQM, namely to calculate visibility impacts, secondary pollutants, such as $SO_4^=$, are the contributing pollutants. After reviewing the algorithms used in the MESOPUFF-II code for calculating the chemical conversion and deposition, the IWAQM considered them simple, but adequate. Therefore, the IWAQM is recommending that they be used, recognizing the following limitations. First, the treatment of the aqueous phase conversion of SO_2 to $SO_4^=$ is likely to be greatly underestimated. Field measurements have indicated that when a plume passes through a non-precipitating cloud that the conversion of SO_2 to $SO_4^=$ can be as high as 100% per hour. The assumed conversion of 3% per hour is, therefore, expected to be an underestimate. The model, however, does not adequately treat the occurrence of non-precipitating clouds. Therefore, the tendency will be to underestimate $SO_4^=$ formation when non-precipitating clouds would be present, with a commensurate overestimation of the primary SO_2 concentration.

Ultimately, when examining Air Quality Related Values (AQRVs), one of the parameters of interest is frequently deposition of $SO_4^=$ and NO_3^-. Also, even when trying to estimate impacts on visibility, an accurate assessment should include the removal of these pollutants from the atmosphere.

Therefore, the IWAQM is recommending that transformation and deposition be actively modeled in order to reasonably estimate the fate of pollutants undergoing long range transport.

The IWAQM recognizes that the chemical and depositional algorithms have not been rigorously tested against field data. Chemical and depositional algorithms do not readily lend themselves to field evaluation due to their dependence on the ambient conditions into which they are emitted and the infeasibility of producing and releasing a unique, chemically active tracer to assess chemical conversion and deposition on a source by source basis. Given these limitations, it is not likely that there will be such data available in the near future. Therefore, proposing to use a technically credible method to estimate the formation and deposition of secondary pollutants, seems appropriate, and is the course recommended by the IWAQM.

To be consistent with the current modeling guidance and to attempt to adequately capture year-to-year variation in meteorological conditions, the IWAQM is recommending that five years of meteorological data be run with the MESOPUFF-II analyses. There are some exceptions to this recommendation, noted below.

One of the weaknesses of the MESOPUFF-II modeling system, identified by the IWAQM, is the lack of treatment of terrain on the air flow and the discontinuities in the mixing height field. A meteorological processor, which uses a diagnostic wind model and smooths out the mixing depth fields, has been identified, but has not yet been thoroughly tested with the MESOPUFF-II, and thus, is not being recommended at this time. When this processor is ready for distribution, Appendix A will be updated to include these enhancements. Until such time, the MESOPUFF-II meteorological processor (MESOPAC) should be used.

5.2.1 Increment and NAAQS Cumulative Long Range Transport Analyses

Sources at distances greater than 50 km from a given receptor should be analyzed with the MESOPUFF-II model, run as described in Appendix A. This includes using the chemical transformation and deposition algorithms. Sources within 50 km of a receptor should be modeled using the appropriate model and model options, as recommended in the *Guideline*. The concentrations from these two analyses should be added on an hour-by-hour, receptor-by-receptor, and pollutant-by-pollutant basis.

There will be occasions when a source will be both nearer and farther than 50 km from receptors in an analysis. It is not intended that such a source be analyzed with both models. In general, the nearer receptors will yield the controlling concentrations for that source, therefore, the appropriate *Guideline* model should generally be run for all receptors, for that source. If, however, it is determined that a particular source, modeled with a steady-state, Gaussian model, is possibly causing an exceedance at a receptor more than 50 km from the source, it is obviously appropriate to model its impacts at that receptor with the long range transport model, to more accurately estimate its impacts. Again, it is expected that a fair degree of professional judgement will need to be exercised in these analyses.

When analyzing impacts in a large Class I area it may be appropriate to divide the steady-state, Gaussian plume analyses into several source groups and use meteorological data appropriate to each source group. For example, if a Class I area is 150 km long, it is unlikely that sources located at opposite ends of the area will experience the same meteorology. Therefore, it may be appropriate to use representative meteorological data sets for each end of the Class I area, particularly since the results will be combined with a model which uses spatially and temporally varying wind fields. The use of multiple meteorological data sets in a steady-state, Gaussian plume modeling analysis is not the recommended approach in the *Guideline*; therefore, this is a matter for the appropriate regulatory agencies and should only be considered on a case-by-case basis in consultation with the appropriate EPA regional office.

As noted previously, it is recommended that both the long range transport model and the steady-state Gaussian model be run with five years of meteorological input data. The exception to this is when the source being permitted is within 50 km of the Class I area and has collected at least one year of on-site meteorological data. If a cumulative impact analysis, which includes sources beyond 50 km, is required, the meteorological period of analysis for both analyses should correspond to the period of on-site meteorological data. If, however, the source being permitted is beyond 50 km from the affected Class I area, then it is recommended that the full five years of data should be run for all analyses.

Combining the results of steady-state Gaussian models with a Lagrangian puff model, such as the MESOPUFF-II, will produce some contrived results. The steady-state model assumes instantaneous transport, whereas the Lagrangian puff model simulates the actual transport time. It may be physically impossible for the emissions from a source modeled with the steady-state model to reach a receptor at the predicted time, given the wind speed. However, steady-state models do not generally accurately predict the time and location of maximum concentrations, but are routinely applied as if they do provide such information. Therefore, while combining the results of two fundamentally different modeling systems is somewhat contrived, it is the only workable approach under the regulatory framework.

5.2.2 Visibility Analyses

The MESOPUFF-II model will be run for all sources, whether nearer or farther than 50 km from a receptor, to provide concentrations of $SO_4^=$ and NO_3^- for visibility calculations. A complete description of the visibility calculations is described in Appendix B.

$SO_4^=$ has been identified as the primary constituent of visibility degradation in the eastern U.S.; organic aerosols and NO_3^- are less important contributors, but a significant species, nonetheless. Therefore, it is critical to have estimates of $SO_4^=$ in order to estimate visibility impacts. Estimates of nitrates are desirable and can be obtained from the long range transport modeling system; estimates of organic aerosols, while more important to total scattering than nitrates in most cases, are not readily estimated by the modeling system. Therefore, organic aerosol concentrations will only be considered as a background concentration for determining regional visibility impacts. The MESOPUFF-II model is capable of producing concentrations of $SO_4^=$ and NO_3^-, whereas the preferred models, listed in the *Guideline* are not. Therefore, the IWAQM is recommending that when a cumulative visibility impact analysis is desired, all sources be modeled with MESOPUFF-II in order to estimate regional haze impacts. It is also important to note that although the application of MESOPUFF-II for short transport distances is questionable the contribution for such sources is relatively unimportant. In many permitting analyses, it is likely that only the source being permitted will be analyzed. Therefore, the MESOPUFF-II analysis will be greatly simplified.

The primary purpose of this analysis is to identify regional haze impacts. Plume blight analyses may need to be performed (EPA, 1988), as well, depending on the location of a source with respect to the Class I area. For sources located more than 50 kilometers from a Class I area, the regional haze analysis will generally be more appropriate. The methods, outlined in Appendix B, are based upon analysis of ambient, speciated fine particulate data, correlated with visibility parameters. Therefore, in order to utilize this method, concentrations of particulate species need to be obtained. The MESOPUFF-II model can provide estimates of $SO_4^=$ and NO_3^-, but assumptions need to be included with respect to the cations associated with these radicals in the fine particulate, the amount of primary carbon particles in the atmosphere, and the formation of secondary organic particles. These are documented in Appendix B.

5.2.3 Analysis of Other AQRVs

The modeling system, described herein, will only provide estimates of the ambient concentrations of pollutants or the depositional loadings at given locations. This modeling system is adequate for providing such estimates, which then may be used to assess the total or incremental impacts of these concentrations or depositional loadings on aquatic and terrestrial ecosystems. The methods for estimating effects on these other AQRVs are not provided; such methods should be determined in consultation with the appropriate Federal Land Manager.

5.2.4 Analysis of Primary Emissions of Fine Particulates

The MESOPUFF-II model is not set up to directly simulate emissions of primary particulates. It can, however, be used for such an analysis, although it must be run as an independent simulation from other pollutants of interest. The method for simulating primary emissions of fine particulates follows.

The MESOPUFF-II dispersion model includes the option for modeling primary emissions of $SO_4^=$. Hence, since these are in particulate form, $SO_4^=$ can be used as a surrogate for the emissions of other fine particulate species. If the model is run simulating only $SO_4^=$ emissions, with the chemistry options turned off, an estimate of the ambient concentrations of primary particulate species can be obtained. The deposition algorithms for particulate $SO_4^=$ can be used for other fine particulates, as well. Since the MESOPUFF-II does not include a provision for gravitational settling, ambient concentrations of the course particle fraction (diameters > 2.5 μm) may be overestimated over transport distances greater than 50 km.

6. SUMMARY

The IWAQM considered two Lagrangian puff models for use in regional scale modeling analyses, the MESOPUFF-II and the ARM3. Both models have known limitations. After comparison and examination of the models, it was determined that the ARM3 contained a number of fundamental coding errors which rendered its use suspect. Although the errors are correctable, they invalidate previous evaluation analyses completed with the ARM3. The MESOPUFF-II has been shown to be applicable, on a theoretical basis, for long range transport; has been evaluated with adequate data bases; and has been shown to not be biased toward underestimation. Therefore, the IWAQM is recommending the use of the MESOPUFF-II for long range transport analyses, in the interim, until a more suitable model construct can be developed.

It would be desirable to be able to recommend a single modeling approach for estimating regional impacts on the NAAQS and PSD increments, that is, have a single model which could treat source-receptor distances of less than and greater than 50 km. Given the need for regulatory consistency, it was determined that for calculating impacts on quantities regulated under the Clean Air Act, techniques identified in the *Guideline on Air Quality Models (Revised)* (EPA, 1986) should be used for source-receptor distances of less than 50 km. The MESOPUFF-II model should be run for source-receptor distances greater than 50 km and the results of these two techniques should be added together.

A technique to estimate visibility impacts, based upon statistical relationships between observed fine particle concentrations and visibility parameters, has been provided. The most important constituents in these calculations are the concentrations of sulfate and the relative humidity. The modeling techniques, recommended above, will yield concentration estimates of sulfate and nitrate and the meteorological fields, used as input to the long range transport model, contain the relative humidity. Therefore, the recommended long range transport model can be used to estimate the impacts of pollutant sources on regional visibility degradation.

The recommendations for the use of the long range transport model include the calculation of the chemical conversion of SO_2 and NO_X, and deposition. This is being recommended whether the model is being applied to a PSD increment analysis or to an AQRV analysis. It is recognized that including these processes will decrease the amount of SO_2 calculated by the model, and hence, reduce the calculated increment concentration. However, these processes are known to occur over the long range transport distances being modeled here and their inclusion in the modeling is considered to be critical for an accurate estimation of impacts. Furthermore, in an AQRV analysis, the secondary pollutants generated and removed through these processes are frequently of most concern.

A number of limitations were identified in the recommended modeling system. As improvements become available, it is intended that they be incorporated into the system.

The IWAQM recognizes that by proposing the use of a Lagrangian puff model for use in the interim, it is not possible to guarantee that the results will be more restrictive than more sophisticated techniques to be proposed during Phase 2 of the IWAQM work plan. The IWAQM still asserts, however, that the interim system is the best of currently available alternatives for simulating the impacts of long range transport on the PSD increments, NAAQS, and AQRVs.

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Appendix A

IWAQM Recommendations for Running The MESOPUFF-II Modeling System

IWAQM RECOMMENDATIONS FOR RUNNING THE MESOPUFF-II MODELING SYSTEM

The MESOPUFF-II modeling system was designed to include flexibility in its use, so it could be used to simulate a wide variety of conditions. Therefore, a number of user specifiable parameters were included as input to the system. Furthermore, the MESOPUFF-II modeling system is capable of simulating varying spatial and temporal scales, which also need specification. The purpose of the recommendations contained in this appendix is to provide consistent, technically credible methods for operating the MESOPUFF-II modeling system for regulatory applications. These recommendations refer to model specific variables and options without detailed definition of the options. The user is referred to the MESOPUFF-II user's manual for further information, where needed.

The primary focus of these recommendations is for the evaluation of air pollution impacts on Class I areas, both increment consumption and the impacts on Air Quality Related Values (AQRVs), from sources located more than 50 kilometers from the potentially affected area. The general procedures outlined could also be used for the assessment of pollution impacts, for source-receptor distances greater than 50 km, outside of Class I areas. The applicability of such techniques should, however, be confirmed with the appropriate regulatory authorities.

Other documents which may be useful to the users of these recommendations include:

User's Guide to the MESOPUFF-II Model and Related Processor Programs, (EPA-600/8-84-013).

A Modeling Protocol for Applying MESOPUFF-II to Long Range Transport Problems, (EPA-454/R-92-021).

Development of the MESOPUFF-II Dispersion Model, (EPA-600/3-84-057).

Spatial Scale

The MESOPUFF-II modeling system is generally applicable to source-receptor distances greater than 50 kilometers. The grid dimensions used in the MESOPUFF-II system, upon which the meteorological fields are defined and the puff calculations are performed, should not exceed 1000 km in the east-west direction or 600 km in the north-south direction (EPA-454/R-92-021). With grid distances greater than this, significant errors can be introduced through the orthogonal nature of the modeling grid, superimposed on the curved surface of the earth. The computational grid size should be such that sources and receptors of interest are not too close to the edge of the grid, since once puffs leave the grid, they are eliminated from the computations; concentrations may be significantly underestimated for sources or receptors too close to the edge of the computational grid.

Spatial Resolution

The various grid systems used in the MESOPUFF-II modeling system are all relative to the initially defined meteorological grid. Therefore, the resolution (grid spacing) of the meteorological grid is of prime importance. Since the meteorological fields, generated by the MESOPAC processor, are defined from the interpolation of available observations, the practical resolution of those fields will depend on the distance between observation stations. Therefore, the maximum recommended resolution is $\frac{1}{3}$ the median distance between observation stations. Finer resolutions can be used, but at the cost of some computation time. If an area in the domain is considered very important and has relatively dense meteorological observations, then the resolution should be based on this area of more refined observations.

In general, all available meteorological stations within the initially defined grid system should be included in the analysis. Stations relatively near to the boundaries, particularly upper air stations, should also be included, as they will improve the representativeness of the wind fields generated by the interpolation.

Temporal Scale

In order to capture year-to-year meteorological variability and the effect that can have on air pollution concentrations, five years of meteorological data should be run with the MESOPUFF-II modeling system.

Precipitation and Upper Air Meteorological Processors

The version of MESOPAC, the meteorological processor for the MESOPUFF-II modeling system, being distributed, can make use of upper-air meteorological data in either a TD-5600 format or the newer TD-6201 format. Processors for both of these data types are provided with the modeling system. Precipitation data is now distributed in a TD-3240 format. Descriptions and information on running these processors are provided below.

User Instructions - Preprocessor Programs

READ56/READ62 Upper Air Preprocessors

READ56 and READ62 are preprocessing programs which extract and process upper air wind and temperature data from standard

NCDC data formats into a form required by the MESOPAC meteorological model. READ56 operates on the older TD-5600 data format. Although this format is not currently used by NCDC, many historical data sets contain data in this format. READ62 processes data in the current TD-6201 format.

Although the data inputs are different, the user inputs to the program are identical as is the processed output file. In the user input file, the user selects the starting and ending dates of the data to be extracted and the top pressure level. Also selected are processing options determining how missing data are treated. The programs will flag or eliminate sounding levels with missing data.

If the user selects the option to flag (rather than eliminate) levels with missing data, the data field of the missing variables are flagged with a series of nines. If the option to eliminate levels with missing data is chosen, only sounding levels with all values valid will be included in the output data file.

Although MESOPAC allows missing values of wind speed, wind direction, and temperature at intermediate levels (i.e., levels other than the surface and model top), the user is cautioned against using soundings with significant gaps due to missing data. For example, adequate vertical resolution of the morning temperature structure near the surface is especially important to the model for predicting daytime mixing heights. It should be kept in mind that the model will fill in missing data by assuming that a straight-line interpolation between valid levels is appropriate. If this assumption is questionable, the sounding should not be used with the model.

Two input files are required by the preprocessor: a user input control file and the NCDC upper air data file. Two output files are produced: a list file summarizing the user option selected and missing data monitored and the processed data file in MESOPAC format. Table A-1 contains a listing of the input and output files for READ56 and READ62.

The READ56/READ62 control file consists of two lines of data entered in FORTRAN free format. A description of each input variable is shown in Table A-2. A sample input file is shown in Table A-3.

The output data file (UP.DAT) produced by READ56/READ62 is a formatted file containing the pressure, elevation, temperature, wind speed, and wind direction at each sounding level. The contents and format of the UP.DAT file are discussed in Section A.2.3.

Table A-1

(a) READ56 Input and Output Files

Unit	File_Name	Type	Format	Description
5	READ56.INP	input	formatted	Control file containing user inputs
6	READ56.LST	output	formatted	List file (line printer output file)
8	TDF56.DAT	input	formatted	Upper air data in NCDC TD-5600 format
9	UP.DAT*	output	formatted	Output file containing processed upper air data in format required by MESOPAC

(b) READ62 Input and Output Files

Unit	File_Name	Type	Format	Description
5	READ62.INP	input	formatted	Control file containing user inputs
6	READ62.LST	output	formatted	List file (line printer output file)
8	TD6201.DAT	input	formatted	Upper air data in NCDC TD-6201 format
9	UP.DAT*	output	formatted	Output file containing processed upper air data in format required by MESOPAC

*Should be renamed UP1.DAT (for upper air station #1), UP2.DAT (for station #2), etc. for input into the MESOPAC model.

Table A-2
READ56/READ62 Control File Inputs

RECORD 1. Starting and ending date/hour, top pressure level to extract.			
Columns	Variable	Type	Description
*	IBYR	integer	Starting year of data to extract (two digits)
*	IBDAY	integer	Starting Julian day
*	IBHR	integer	Starting hour (00 or 12 GMT)
*	IEYR	integer	Ending year of data to extract (two digits)
*	IEDAY	integer	Ending Julian day
*	IEHR	integer	Ending hour (00 or 12 GMT)
*	PSTOP	real	Top pressure level (mb) for which data is extracted (possible values are 850 mb, 700 mb, or 500 mb). The output file will contain data from the surface to the "PSTOP"-mb pressure level.

* Entered in FORTRAN free format

Table A-2 (Concluded)
READ56/READ62 Control File Inputs

RECORD 2. Missing data control variables			
Columns	Variable	Type	Description
*	LHT	logical	Height field control variable. If LHT = T, a sounding level is eliminated if the height field is missing. If LHT = F, the sounding level is included in the output file but the height field is flagged with a "9999", if missing.
*	LTEMP	logical	Temperature field control variable. If LTEMP = T, a sounding level is eliminated if the temperature field is missing. If LTEMP = F, the sounding level is included in the output file but the temperature field is flagged with a "999.9", if missing.

*	LWD	logical	Wind direction field control variable. If LWD = T, a sounding level is eliminated if the wind direction field is missing. If LWD = F, the sounding level is included in the output file but the wind direction field is flagged with a "999", if missing.
*	LWS	logical	Wind speed field control variable. If LWS = T, a sounding level is eliminated if the wind speed field is missing. If LWS = F, the sounding level is included in the output file but the wind speed field is flagged with a "999", if missing.

* Entered in FORTRAN free format

Table A-3
Sample READ56/READ62 Control File (READ56.INP, READ62.INP)

```
79, 365, 00, 80, 002, 00, 500. -- Beg. yr, day, hr(GMT), Ending yr, day, hr, top pressure
level

.TRUE., .TRUE., .TRUE., .TRUE.   -- Eliminate level if height, temp., wind direction, wind
direction, wind speed missing ?
```

PXTRACT Precipitation Data Extract Program

PXTRACT is a preprocessor program which extracts precipitation data for stations and time periods of interest from a fixed length, formatted precipitation data file in NCDC TD-3240 format. Hourly precipitation data is available from NCDC in large blocks of data sorted by station. For example, a typical TD-3240 file for California may contain data from over 100 stations statewide in blocks of time of 30 years or more. Modeling applications require the data sorted by time rather than station, and usually involve limited spatial domains of tens of kilometers or less and time periods of one year or less. PXTRACT allows data for a particular model run to be extracted from the larger data file and creates a set of station files that are used as input files by the second-stage precipitation preprocessor, PMERGE (see PMERGE section)

NOTE: If wet removal is not to be considered by the MESOPUFF-II dispersion model, no precipitation processing needs to be done. PXTRACT (and PMERGE) are required only if wet removal is an important removal mechanism for the modeling application of interest. In addition, if wet removal is a factor, the user has the option of creating a free-formatted precipitation data file that can be read by MESOPAC. This option eliminates the need to run the precipitation preprocessing programs for short MESOPAC runs (e.g., screening runs) for which the input data can easily be input manually.

The input files used by PXTRACT include a control file (PXTRACT.INP) containing user inputs, and a data file (TD3240.DAT) containing the NCDC data in TD-3240 format. The precipitation data for stations selected by the user is extracted from the TD3240.DAT file and stored in separate output files (one file per station) called xxxxxx.DAT, where xxxxxx is the station identification code. PXTRACT also creates an output list file (PXTRACT.LST) which contains the user options and summarizes the station data extracted. Table A-12 contains a summary of PXTRACT's input and output files.

The PXTRACT control file contains the user-specified variables which determine the method used to extract precipitation data from the input data file (i.e., by state, by station, or all stations), the appropriate state or station codes, and the time period to be extracted. A sample PXTRACT control file is shown in Table A-13. The format and contents of the file are described in Table A-14.

The PXTRACT output list file (PXTRACT.LST) contains a listing of the control file inputs and options. It also summarizes the station data extracted from the input TD-3240 data file, including the starting and ending date of the data for each station and the number of data records found. The PXTRACT output data files consist of precipitation data in TD-3240 format for the time period selected by the user. Each output data file contains the data for one station.

Table A-12
PXTRACT Input and Output Files

Unit	File Name	Type	Format	Description
1	PXTRACT.INP	input	formatted	Control file containing user inputs
2	TD3240.DAT	input	formatted	Precipitation data in NCDC TD-3240 format
6	PXTRACT.LST	output	formatted	List file (line printer output file)
7	id1.DAT (id1 is the 6-digit station code for station #1, e.g., 040001)	output	formatted	Precipitation data (in TD-3240) format for station #1 for the time period selected by the user

8	id2.DAT (id2 is the 6-digit station code for station #2, e.g., 040002)	output	formatted	Precipitation data (in TD-3240) format for station #2 for the time period selected by the user
. . . (Up to 200 new precipitation data files are allowed by PXTRACT).				

Table A-13
Sample PXTRACT Control File (PXTRACT.INP)

```
2                              -- Selection code, ICODE
5                              -- Number of states or stations
040001                         -- State or station code
040002
040003
040004
040005
80 01 01 01 80 01 02 24        -- Starting yr, month, day, hour(01-24),
                                  ending yr, month, day, hour
```

Table A-14
PXTRACT Control File Inputs (PXTRACT.INP)

RECORD 1. Data selection code.			
Columns	Variable	Type	Description
*	ICODE	Integer	Selection Code: 1 = extract all stations within state or states requested 2 = input a list of station codes of stations to extract 3 = extract all stations in input file with data for time period of interest

----
* Entered in Fortran free format

Table A-14 (Continued)
PXTRACT Control File Inputs (PXTRACT.INP)

RECORD 2. Number of state or station codes (This record is included only if ICODE = 1 or 2)			
Columns	Variable	Type	Description
*	N	Integer	If ICODE = 1: Number of state codes to follow If ICODE = 2: Number of station codes to follow

----
* Entered in Fortran free format

Table A-14 (Continued)
PXTRACT Control File Inputs (PXTRACT.INP)

RECORD 3, 4, ... 2+N. State or station codes of data to be extracted			
Columns	Format	Variable	Description
1-6	I6	IDAT	If ICODE=1: State code (two digits) If ICODE=2: Station code (six digits) consisting of state code (two digits) followed by station ID (four digits)

Table A-14 (Concluded)
PXTRACT Control File Inputs (PXTRACT.INP)

NEXT RECORD. Starting/ending dates and times			
Columns	Format*	Variable	Description
1-2	I2	IBYR	Beginning year of data to process (two digits)
4-5	I2	IBMO	Beginning month
7-8	I2	IBDAY	Beginning day
10-11	I2	IBHR	Beginning hour (01-24 LST)
13-14	I2	IEYR	Ending year of data to process (two digits)
16-17	I2	IEMO	Ending month
19-20	I2	IEDAY	Ending day
22-23	I2	IEHR	Ending hour (01-24 LST)

----
*Record format is (8(i2,1x)

Table A-16
Sample TD-3240 Format Precipitation Data File (040001.DAT)

```
HPD04000100HPCPHI19820100010010100 00002
HPD04000100HPCPHI19820100010010200 00002
HPD04000100HPCPHI19820100010010300 00004
HPD04000100HPCPHI19820100020010700 00000
HPD04000100HPCPHI19820100030011300 00000M
HPD04000100HPCPHI19820100120010400 00000M
HPD04000100HPCPHI19820100120010500 00000
```

PMERGE Precipitation Data Preprocessor

PMERGE reads, processes and reformats the precipitation data files created by the PXTRACT program, and creates an unformatted data file for input into the MESOPAC meteorological model. The output file (PRECIP.DAT) contains the precipitation data sorted by hour, as required by MESOPAC, rather than by station. The program can also read an existing unformatted output file and add stations to it, creating a new output file. PMERGE also resolves "accumulation periods" and flags missing or suspicious data.

Accumulation periods are intervals during which only the total amount of precipitation is known. The time history of precipitation within the accumulation period is not available. For example, it may be known that within a six-hour accumulation period, a total of a half inch of precipitation fell, but information on the hourly precipitation rates within the period is unavailable. PMERGE resolves accumulation periods such as this by assuming a constant precipitation rate during the accumulation period. For modeling purposes, this assumption is suitable as long as the accumulation time period is short (e.g., a few hours). However, for longer accumulation periods, the use of the poorly time-resolved precipitation data is not recommended. PMERGE will eliminate and flag as missing any accumulate periods longer than a user-define maximum length.

PMERGE provides an option to "pack" the precipitation data in the unformatted output in order to reduce the size of the file. A "zero packing" method is used to pack the precipitation data. Because many of the precipitation values are zero, strings of zeros are replaced with a coded integer identifying the number of consecutive zeros that are being represented. For example, the following record with data from 20 stations requires 20 unpacked words:

0.0, 0.0, 0.0, 0.0, 0.0, 1.2, 3.5, 0.0, 0.0, 0.0,
0.0, 0.0, 0.0, 0.7, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,

These data in packed form would be represented in six words:

-5., 1.2, 3.5, -6., 0.7, -6.

where five zero values are replaced by -5., six zero values are replaced by -6., etc. With many stations and a high frequency of zeros, very high packing ratios can be obtained with this simple method. All of the packing and unpacking operations are performed internally by PMERGE and MESOPAC, and are transparent to the user. The header records of the data file contain information flagging the file to MESOPAC as a packed or unpacked file. If the user selects the unpacked format, each precipitation value is assigned one full word.

The input files used by PMERGE include a control file (PMERGE.INP), an optional unformatted data file (PBIN.DAT) created in a previous run of PMERGE, and up to 150 TD-3240 precipitation station files (e.g., as created by PXTRACT). The output file consists of a list file and a new unformatted data file in MESOPAC format with the data for all stations sorted by hour. Table A-17 lists the name, type, format, and contents of PMERGE's input and output data files.

The PMERGE control file (PMERGE.INP) contains the user-specified input variables indicating the number of stations to be processed, a flag indicating if data is to be added to an existing, unformatted data file, the maximum length of an accumulation period, packing options, station data, and time zone data. PMERGE allows data from different time zones to be merged by time-shifting the data to a user-specified base time zone. A sample PMERGE control file is shown in Table A-18. The format and contents of the file are described in Table A-19.

The PMERGE output list file (PMERGE.LST) contains a listing of the control file inputs and options. It also summarizes the number of valid and invalid hours for each station including information on the number of hours with zero or non-zero precipitation rates and the number of accumulative period hours. Additional statistics provide information by station on the frequency and type of missing data in the file (i.e., data flagged as missing in the original data file, data which is part of an excessively long accumulation period, or data missing from the input files before (after) the first (last) valid record.

Table A-17

PMERGE Input and Output Files

Unit	File_Name	Type	Format	Description
3	PBIN.DAT	input	unformatted	Existing PMERGE data file to which stations are to be added (Used_only_if_NBF=1)
4	PRECIP.DAT	output	unformatted	Output data file created by PMERGE (PRECIP.DAT is an input file to MESOPAC)
5	PMERGE.INP	input	formatted	Control file containing user inputs
6	PMERGE.LST	output	formatted	List file (line printer output file)
7	user input file name	input	formatted	Precipitation data (in TD-3240) format for station #1. (Output file of PXTRACT)
8	user input file name	input	formatted	Precipitation data (in TD-3240) format for station #2. (Output file of PXTRACT)
. . . (Up to 150 new precipitation data files are allowed by PMERGE).				

Table A-18
Sample PMERGE Control File (PMERGE.INP)

```
   5   0  12   5   2   0      -- No. stations,no. binary files,max. accum. period,base time
                                      zone,ioform(1=binary,2=formatted),pack(0=no, 1=yes) --
(6I4)
040001.dat  5                 -- Input file name, time zone         -- (A10,I3)
040002.dat  5                  "    "    "     "    "
040003.dat  5                  "    "    "     "    "
040004.dat  5                  "    "    "     "    "
040005.dat  5                  "    "    "     "    "
```

82 01 01 01 82 01 03 01   -- Starting yr, month, day, hour (01-24), ending yr, month, day, hour (01-24)
-- (8(I2,1X))

Table A-19
PMERGE Control File Inputs (PMERGE.INP)

RECORD 1. General run information.			
Columns	Format*	Variable	Description
1-4	I4	NFF	Number of formatted 80-column NCDC input files to be processed (up to 150)
5-8	I4	NBF	Flag indicating if data is to be added to an existing unformatted precip. data file (0=no, 1=yes)
9-12	I4	MAXAP	Maximum allowed length of an accumulation period (hours). It is recommended that MAXAP be set to 24 hours or less.
13-16	I4	IOTZ	Time zone of output data (05=EST, 06=CST, 07=MST, 08=PST)
17-20	I4	IOPACK	Flag indicating if output data are to be packed (0=no, 1=yes)

----

*Record format is (5i4)

Table A-19 (Continued)
PMERGE Control File Inputs (PMERGE.INP)

RECORDS 2, 3, ... 1+NFF. File names and time zone of each station (Each_record_has_the_following_format)			
Columns	Format*	Variable	Description
1-10	A10	CFFILES	Name of file containing formatted precipitation data (TD-3240 format) (PXTRACT output file). First six digits of file name must contain station code (SSIIII), where SS is the two digit state code, and IIII is the station ID)
12-13	I2	ISTZ	Time zone of station (08=PST)

Record format is (a10,1x,i2)

Table A-19 (Concluded)
PMERGE Control File Inputs (PMERGE.INP)

NEXT RECORD. Starting/ending dates and times			
Columns	Format*	Variable	Description
1-2	I2	IBYR	Beginning year of data to process (two digits)
4-5	I2	IBMO	Beginning month
7-8	I2	IBDAY	Beginning day
10-11	I2	IBHR	Beginning hour (01-24 LST)
13-14	I2	IEYR	Ending year of data to process (two digits)
16-17	I2	IEMO	Ending month
19-20	I2	IEDAY	Ending day
22-23	I2	IEHR	Ending hour (01-24 LST)

Record format is (8(i2,1x))

MESOPAC Input Fields

The version of MESOPAC discussed herein, includes some enhancements from earlier versions. These include an expanded format for including precipitation data (TD-3240) and the inclusion of site specific data on the wind speed measurements, specifically the wind speed measurement height and the surface roughness length appropriate for the surface station site. Inclusion of the TD-3240 requires running the precipitation processors described previously. Some coding enhancements were implemented to trap artifacts, produced by the model, and treat them in a consistent manner.

Card Group 1 - TITLE				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-80	CA	title(20)	80 Character Title	Appropriate Choice

Card Group 2 - GENERAL RUN INFORMATION

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	I	nyr	Two Digit Year	Appropriate Choice
6-10	I	idystr	Starting Julian Day	Appropriate Choice
11-15	I	ihrmax	Number of Hours in Run	Appropriate Choice
16-20	I	nssta	# Surface Stations	≤ 25
21-25	I	nusta	# Rawinsonde Stations	≤ 10
26-30	I	ibtz	Reference Time Zone	5=EST 6=CST 7=MST 8=PST
31-35	I	npsta	# Precipitation Stations	≤ 200

Card Group 3 - GRID DATA

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	I	imax	# X grid points (west-east)	≤ 40
6-10	I	jmax	# Y grid points (south-north)	≤ 40
11-20	R	dgrid	grid spacing (m)	⅓ median distance between stations

Card Group 4 - OUTPUT OPTIONS

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	L	lsave	Binary To Disk for Post-processing	T
6-10	L	lprint	Print Met fields	F (can produce voluminous output)
11-15	I	iprint	Print Interval (hours)	≥ 1 (used only if lprint=T)
16-20	L	lbd	Print Met Input	F (can produce voluminous output)
21-25	I	ndy1	Julian day to start printing input	(used only if lbd=T)
26-30	I	nhr1	Hour to start printing input	(used only if lbd=T)
31-35	I	ndy2	Julian day to stop printing input	(used only if lbd=T)
36-40	I	nhr2	Hour to stop printing input	(used only if lbd=T)

Card Group 5 - GRIDDED LAND USE CATEGORIES

Columns	Typ*	Variable Name	Description	Recommended Value
1-80 Format (40i2)	IA	Ilandu (40,40)	Land use categories for each grid point	As Appropriate

'jmax' cards are required, each card with 'imax' land use categories (corresponding to X-coordinates 1 to imax). The first card contains values for Y = jmax, the second card for Y = jmax-1, etc.

Card Group 6 - DEFAULT OVERRIDE OPTIONS

Columns	Typ*	Variable Name	Description	Recommended Value
1	IAE	iopts(1)	Use Default Surface Wind Speed Measurement Height (Default=10m)	0
2	IAE	iopts(2)	Use Default von Karman Constant (Default=0.4)	0
3	IAE	iopts(3)	Use Default Friction Velocity Constants (Defaults: γ=4.7, A=1100)	0
4	IAE	iopts(4)	Use Default Mixing Height Constants (Defaults: B=1.41, E=0.15, Δz=200m, $\partial\theta/\partial z_{min}$=0.001°K/m, N=2400	0
5	IAE	iopts(5)	Use Default Wind Field Variables (Defaults: Vertically Averaged Winds used from Ground to Mixing Height, Vertically Averaged Winds used from Mixing Height to 700 mb, & Scan Radius for Wind Field Interpolation RADIUS=99.0km)	0
6	IAE	iopts(6)	Use Default Surface Roughness Lengths (Determined from Land Use Categories)	0
7	IAE	iopts(7)	Use Default Heat Flux Estimates (Can not be changed)	0

8	IAE	iopts(8)	Use Default Radiation Reduction Factors (Defaults: 1.0, 0.91, 0.84, 0.79, 0.75, 0.72, 0.68, 0.62, 0.53, 0.41, 0.23	0
9	IAE	iopts(9)	Use Default Heat Flux Constants (Default: RADC=0.3)	0
10	IAE	iopts(10)	If iopts(10)=1, starting date of run is <u>not</u> the beginning of the meteorological file, else set iopts(10)=0	0 or 1 as appropriate

<u>Card Groups 7-14</u> - NEW VALUES TO REPLACE DEFAULT PARAMETERS

The default options are recommended for all regulatory uses of the MESOPUFF-II modeling system. If the defaults are used, these card groups do not need to be included. See the user's manual for further information.

<u>Card Group 15</u> - SURFACE STATION DATA. 'nssta' cards - one for each CD144/TD9657 surface station

Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	IAE	idcd	Surface station ID for CD144 data (5 digits)	As Appropriate
6-15	RAE	xscoor	X-coordinate of station (in grid units)	As Appropriate
16-25	RAE	yscoor	Y-coordinate of station (in grid units)	As Appropriate
26-35	RAE	slat	Station latitude (decimal degrees)	As Appropriate
36-45	RAE	slong	Station longitude (decimal degrees)	As Appropriate
46-50	RAE	szone	Station time zone (5=EST 6=CST 7=MST 8=PST)	As Appropriate
51-55	IAE	isunit	Logical unit number of CD144 surface data	As Appropriate
56-65	IAE	idprcp	Surface station ID for TD9657 data (6 digits)	<u>TD9657 data not implemented in this</u> version

66-70	IAE	ipunit	Logical unit number of TD9657 data (ipunit=999 if TD9657 data is not available for this station)	999 TD9657 data not implemented in this version
71-75	R	zmsurf	Wind measurement height at station idcd (m)	As Appropriate
76-80	R	z0surf	Surface Roughness Length (m) for surface station site	As Appropriate

Card Group 16 - RAWINSONDE STATION DATA. 'nusta' cards - one for each TDF5600 or TDF6201 rawinsonde station.

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	IAE	idtd	Rawinsonde station identification number (5 digits)	As Appropriate
6-15	RAE	xucoor	X-coordinate of station (in grid units)	As Appropriate
16-25	RAE	yucoor	Y-coordinate of station (in grid units)	As Appropriate
26-35	RAE	ulat	Station latitude (decimal degrees)	As Appropriate
36-45	RAE	ulong	Station longitude (decimal degrees)	As Appropriate
46-50	RAE	uzone	Station time zone (5=EST 6=CST 7=MST 8=PST)	As Appropriate
51-55	IAE	iuunit	Logical unit of processed TDF5600 or TDF6201 data	As Appropriate

Card Group 17 - PRECIPITATION STATION DATA. 'npsta' cards - one for each precipitation station.				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	IAE	idp	Precipitation station IDs	As Appropriate
6-15	RAE	xpcoor	X-coordinate (grid units)	As Appropriate
16-25	RAE	ypcoor	Y-coordinate (grid units)	As Appropriate

* The codes under type correspond to the following:
I Integer Variable
IA Integer Array
IAE Integer Array Element
R Real Variable
RA Real Array
RAE Real Array Element
C Character Variable
CA Character Array
L Logical Variable

MESOPUFF-II Input Fields

The version of the MESOPUFF-II described below contains some enhancements from earlier versions. These allow for the initialization of runs from the results of previous runs and the output of deposition calculations, both wet and dry.

Some modifications to the modeling code were implemented to make some of the default values consistent with those recommended here, and to make some of the calculations, such as plume rise, consistent with the methods implemented in EPA's preferred models.

Card Group 1 - TITLE				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-80	CA	title(20)	80 Character Title	Appropriate Choice

Card Group 2 - GENERAL RUN INFORMATION				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	I	nsyr	Two digit year of run	As Appropriate
6-10	I	nsday	Starting Julian day	As Appropriate
11-15	I	nshr	Starting Hour	(00-23)
16-20	I	nadvts	Number of hours in run	As Appropriate
21-25	I	npts	# point sources	(≤ 20)
26-30	I	nareas	# area sources	(≤ 5)
31-35	I	nrec	# non-gridded receptors	(≤ 180)
36-40	I	npec	# of chemical species to model (=1 SO_2 $\mid$ =2 SO_2 & $SO_4^=$ $\mid$ =3 SO_2, $SO_4^=$, & NO_x $\mid$ =5 SO_2, $SO_4^=$, NO_x, HNO_3, & NO_3^-	2 if SO_2 Source 5 if SO_2 and NO_x source
41-45	I	icont	Continuation run (0=no, 1=yes)	As Appropriate

Card Group 3 - COMPUTATIONAL VARIABLES				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	I	iavg	Concentration averaging time (hours)	1
6-10	I	npuf	Puff Release Rate (puffs/hour)	4
11-15	I	nsamad	Minimum Sampling Rate (samples/hour)	2
16-20	L	lvsamp	Variable Sampling Option (T or F)	T
21-25	R	wsamp	Reference wind speed for variable sampling	2.
26-30	L	lsgrid	Calculate gridded concentrations at sampling grid points	As Appropriate (T or F)
31-35	R	agemin	Minimum age of puffs to sample (seconds)	900.

Card Group 4 - GRID INFORMATION				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	I	iastar	Element # of the meteorological grid defining the beginning	(1≤iastar≤imax, where imax=met grid size from MESOPAC)

6-10	I	iastop	Element # of the meteorological grid defining the end of the computational grid in the X-direction	(1≤iastop≤imax)
11-15	I	jastar	Element # of the meteorological grid defining the beginning of the computational grid in the Y-direction	(1≤jastar≤jmax, where jmax=met grid size from MESOPAC)
16-20	I	jastop	Element # of the meteorological grid defining the end of the computational grid in the Y-direction	(jastar≤jastop≤jmax)
21-25	I	isastr	Element # of the meteorological grid defining the beginning of the sampling grid in the X-direction	(1≤isastr≤iastar)
26-30	I	isastp	Element # of the meteorological grid defining the end of the sampling grid in the X-direction	(isastr ≤ isastp ≤ iastop)
31-35	I	jsastr	Element # of the meteorological grid defining the beginning of the sampling grid in the Y-direction	(1≤jsastr≤jastar)
36-40	I	jsastp	Element # of the meteorological grid defining the end of the sampling grid in the Y-direction	(jsastr ≤ jsastp ≤ jastop)
41-45	I	meshdn	Sampling grid spacing factor	The sample grid spacing ≡ dgrid/meshdn, where dgrid = met grid spacing (m)

Card Group 5 - TECHNICAL OPTIONS

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	L	lgauss	Vertical Distribution control (F=uniform, T=Gaussian)	T
6-10	L	lchem	Chemical transformation control	T
11-15	L	ldry	Dry deposition control	T
16-20	L	lwet	Wet removal control	T
21-25	L	l3vl	Dry removal from surface layer (T) or throughout mixed layer (F)	T

Card Group 6 - OUTPUT OPTIONS

Columns	Typ*	Variable Name	Description	Recommended Value
1-5	L	lsave	Disk/tape output	Generally true (T) (allows post-analysis)
6-10	L	lprint	Print concentrations	Generally false (F) (will usually want some other averaging times, so will use results from post-analysis)
11-15	I	iprint	Print interval in hours of concentrations	(Used only if lprint=T)
16-20	L	lbd	Print puff data (puff height, σ_y, σ_z, location, transformation rate, etc.	Generally false (F) (can produce voluminous output)
21-25	I	nn1	Time step to begin printing puff data	Generally 0 (if lbd=T, then $1 \leq nn1 \leq nadvts$)
26-30	I	nn2	Time step to stop printing puff data	Generally 0 (if lbd=T, then $nn1 \leq nn2 \leq nadvts$)
31-35	L	lwetg	Wet flux at gridded receptors	T if gridded receptors used
36-40	L	lwetng	Wet flux at non-gridded receptors	T if non-gridded receptors used
41-45	L	ldryg	Dry flux at gridded receptors	T if gridded receptors used

46-50	L	ldryng	Dry flux at non-gridded receptors	T if non-gridded receptors used
51-55	L	lsavef	Save wet/dry fluxes	T (allows for post-processing)
56-60	L	lprflx	Print wet/dry fluxes	F (can create voluminous output)
61-65	I	ires	Save results for restart?	0=no, 1=yes Generally 1
66-70	I	iint	Save results every 'iint' hours and the last hour of the run	9999 saves only last hour for restart

Card Group 7

Columns	Typ*	Variable Name	Description	Recommended Value
1	IAE	iopts(1)	Use default dispersion parameters (a_y, b_y, a_z, b_z, a_{zt} as defined by Turner and Heffter, T_m=10000, jsup=5 (T_m reset in code from original default value of 100000)	0
2	IAE	iopts(2)	Use default vertical diffusivity constants k_1=0.01, k_2=0.10	0
3	IAE	iopts(3)	Use default SO_2 canopy resistance	0
4	IAE	iopts(4)	Use default dry deposition parameters	0
5	IAE	iopts(5)	Use default wet removal parameters	0
6	IAE	iopts(6)	Use default chemical transformation methods	0

Card Groups 8-13 - NEW VALUES TO REPLACE DEFAULT PARAMETERS

The default options are recommended for all regulatory uses of the MESOPUFF-II modeling system. If the defaults are used, these card groups do not need to be included. See the user's manual for further information.

Card Group 14 - POINT SOURCE DATA. 'npts' cards required - one for each point source.				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	RAE	xstak	X-coordinate of point source (in meteorological grid units)	As Appropriate
6-10	RAE	ystak	Y-coordinate of point source (in met grid units)	As Appropriate
11-15	RAE	htstak	Stack height (m)	As Appropriate
16-20	R	d	Stack diameter (m)	As Appropriate
21-25	R	w	Stack exit velocity (m/s)	As Appropriate
26-30	R	tstak	Stack gas temperature (°K)	As Appropriate
31-80	RAE	emis(1-5)	Emission rates (g/s) for SO_2, $SO_4^=$, NO_x, HNO_3, & NO_3^-	As Appropriate

Card Group 15 - AREA SOURCE DATA. 'nareas' cards required - one for each area source.				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-5	RAE	xar	X-coordinate of area source center (in meteorological grid units)	As Appropriate
6-10	RAE	yar	Y-coordinate of area source center (in met grid units)	As Appropriate
11-15	RAE	htar	Effective height of area source (m)	As Appropriate
16-20	RAE	sigyar	Initial σ_y (m) of area source emissions	As Appropriate
21-25	RAE	sigzar	Initial σ_z (m) of area source emissions	As Appropriate
26-75	RAE	emisar (1-5)	Emission rates (g/s) for SO_2, $SO_4^=$, NO_x, HNO_3, & NO_3^-	As Appropriate

Card Group 16 - NON-GRIDDED RECEPTOR COORDINATES. 'nrec' cards required - one for each non-gridded receptor				
Columns	**Typ***	**Variable Name**	**Description**	**Recommended Value**
1-10	RAE	xrec	X-coordinate of non-gridded receptor (in meteorological grid units)	As Appropriate
11-20	RAE	yrec	Y-coordinate of non-gridded receptor (in met grid units)	As Appropriate

* The codes under type correspond to the following:

- I Integer Variable
- IA Integer Array
- IAE Integer Array Element
- R Real Variable
- RA Real Array
- RAE Real Array Element
- C Character Variable
- CA Character Array
- L Logical Variable

Appendix B

Method for Calculating Regional Visibility Impairment

METHOD FOR CALCULATING REGIONAL VISIBILITY IMPAIRMENT

The primary sources of anthropogenically induced, regional visibility degradation (also referred to as regional haze), measured as light extinction, are fine particles (diameters ≤ 2.5 µm) in the atmosphere. In the eastern U.S., these anthropogenic particles are composed primarily of sulfate ($SO_4^=$) compounds, organic compounds, and to a much lesser extent, nitrate (NO_3^-) compounds. These are important constituents in other areas of the U.S. as well; their relative importance, however, changes. For example, in some areas of the Pacific Northwest, organic aerosols are as, or more, important than $SO_4^=$ aerosols. In some parts of Southern California, NO_3^- aerosols are the dominant specie. When examining individual source's or groups of sources' impacts on regional visibility degradation, primary emissions of fine particulate should also be considered.

The generally observed sulfate compound is ammonium sulfate {$(NH_4)_2SO_4$}, although ammonium bisulfate and un-neutralized sulfuric acid particles have also been measured. Particles composed of nitrate compounds usually take the form of ammonium nitrate {NH_4NO_3}. These compounds are generally not directly emitted from air pollutant sources, but are formed through a series of chemical reactions in the atmosphere. The air pollutants, which contribute to the formation of these particles, are gaseous emissions of oxides of sulfur and nitrogen (SO_X and NO_X), which eventually oxidize to form $SO_4^=$ and nitric acid (HNO_3), as well as other compounds, and utlimately react with natural and anthropogenic emissions of ammonia. The formation of NH_4NO_3 is dependent on the concentrations of ammonia gas (NH_3) and nitric acid (HNO_3) as well as the concentration of $SO_4^=$. $SO_4^=$ competes with HNO_3 for the available NH_3. Thus, in the presence of both $SO_4^=$ and HNO_3, $(NH_4)_2SO_4$ will be formed preferentially to NH_4NO_3. Essentially, NH_4NO_3 will only be formed when there is an excess of NH_3 available, relative to $SO_4^=$. The MESOPUFF-II modeling system accounts for the balance between $SO_4^=$, HNO_3 and NH_3. Therefore, emissions of both SO_2 and NO_X should be modeled in the same run to account for this balance. This balance will not be accounted for if Level I methods are used; the contribution of NO_3^- to visibility degradation may be overestimated in Level I analyses, but this is consistent with the rationale for Level I.

As noted above, fine particles are the major contributor to anthropogenically produced visibility degradation, and sulfates and organics constitute the highest contributions to measured fine particle concentrations in most areas of the country. Organic aerosols are generally considered to be secondary products of chemical reactions in the atmosphere; the processes which lead to their formation are not well understood. The sources of organic aerosols can be both natural and anthropogenic. Current modeling and analysis techniques are inadequate for providing an estimate of organic aerosols.

Thus, for the purposes of calculating regional visibility degradation due to specific sources of air pollution, the primary focus will be on the contribution to light extinction of fine particles of sulfate compounds and nitrate compounds, expressed as $(NH_4)_2SO_4$ and NH_4NO_3. Once these particles are formed, however, their size can change, and thus their light scattering efficiency, due to changes in the relative humidity of the atmosphere. Therefore, in order to adequately account for the contribution to light extinction of either $(NH_4)_2SO_4$ or NH_4NO_3 the mass of these constituents and the relative humidity of the atmosphere in which these particles reside must be known. The calculations of the extinction due to primary fine particulates are assumed to be non-hygroscopic.

Method

1. Apply an appropriate air quality model to obtain hourly concentrations of $SO_4^=$ and/or NO_3^- and/or primary fine particulate.
    a. If using MESOPUFF-II concentrations of $SO_4^=$ and NO_3^- are obtained as direct model output (refer to Appendix A).
        1) To obtain primary fine particulate concentrations, The MESOPUFF-II should be run as an independent run from the $SO_4^=$ and NO_3^- run, assuming all of the fine particulate emissions are $SO_4^=$ emissions and that they are the only emissions in that run, the chemistry options should be turned off, and the deposition options should be turned on. The other options should be set as described in Appendix A.
    b. If running a steady-state model, use the methods, outlined in Inset 1 of the main body of the report, to convert SO_x and NO_x to $SO_4^=$ and NO_3^-. The primary fine particulate emissions can be directly modeled.

2. As noted above, it is assumed that the compounds of concern are $(NH_4)_2SO_4$ and NH_4NO_3 and primary fine particulate. Therefore the mass concentrations of $SO_4^=$ and NO_3^- must be corrected for the presence of NH_4^+. (The primary fine particulate is modeled as $SO_4^=$, as a surrogate in MESOPUFF-II; this should <u>not</u> be corrected for NH_4^+.)
    a. Multiply the mass concentration of $SO_4^=$ by 1.375 to obtain $(NH_4)_2SO_4$

b. Multiply the mass concentration of NO_3^- by 1.29 to obtain $NH_4NO_3$1. Obtain the hourly values of relative humidity, appropriate for each receptor and corresponding to the hourly concentrations calculated in step 1.

c. These can be obtained from the MESOPUFF-II meteorological files.

d. If hourly relative humidity values are not available, assume that the relative humidity is 95%.

e. Obtain the relative humidity correction factor (*f(RH)*) from Figure B-1 (see also Table B-1).

3. Calculate the extinction based on the following equation.

$$b_{ext.s} = 0.003[part]f(RH)$$

$$\text{where}\begin{cases} b_{ext.s} & = \textit{The extinction coefficient due to particle scattering } (km^{-1}) \\ 0.003 & = \textit{a nominal dry scattering efficiency} \\ [part] & = \textit{The concentration of } (NH_4)_2SO_4 \textit{ or } NH_4NO_3 \textit{ in } \mu g/m^3 \\ & \quad \textit{or of primary particulate expressed as } SO_4^= \ (\mu g/m^3) \\ f(RH) & = \textit{The RH correction factor (see figure B-1)} \end{cases}$$

(The dry efficiency is a consensus value based on Trijonis *et al.* (1987) and the relative humidity correction factor is based on Tang *et al.* (1981).)

a. It is only appropriate to compute the extinctions based on hourly values of [part] and relative humidity. It is <u>not</u> appropriate to use average values of these quantities.

b. To calculate the extinction due to primary fine particulate, use the above equation, but set the relative humidity correction factor (*f(RH)*) equal to 1.

Example

If one has a sulfate concentration [$SO_4^=$] of 1.7 μg/m^3, then this would correspond to an ammonium sulfate concentration [$(NH_4)_2SO_4$] of 2.34 μg/m^3. The extinction due to this concentration would be 0.003×2.34×*f(RH)* km^{-1}. From Figure B-1, if the relative humidity is 95%, *f(RH)* is 11.5. Therefore $b_{ext.s}$ = 0.08 km^{-1}.

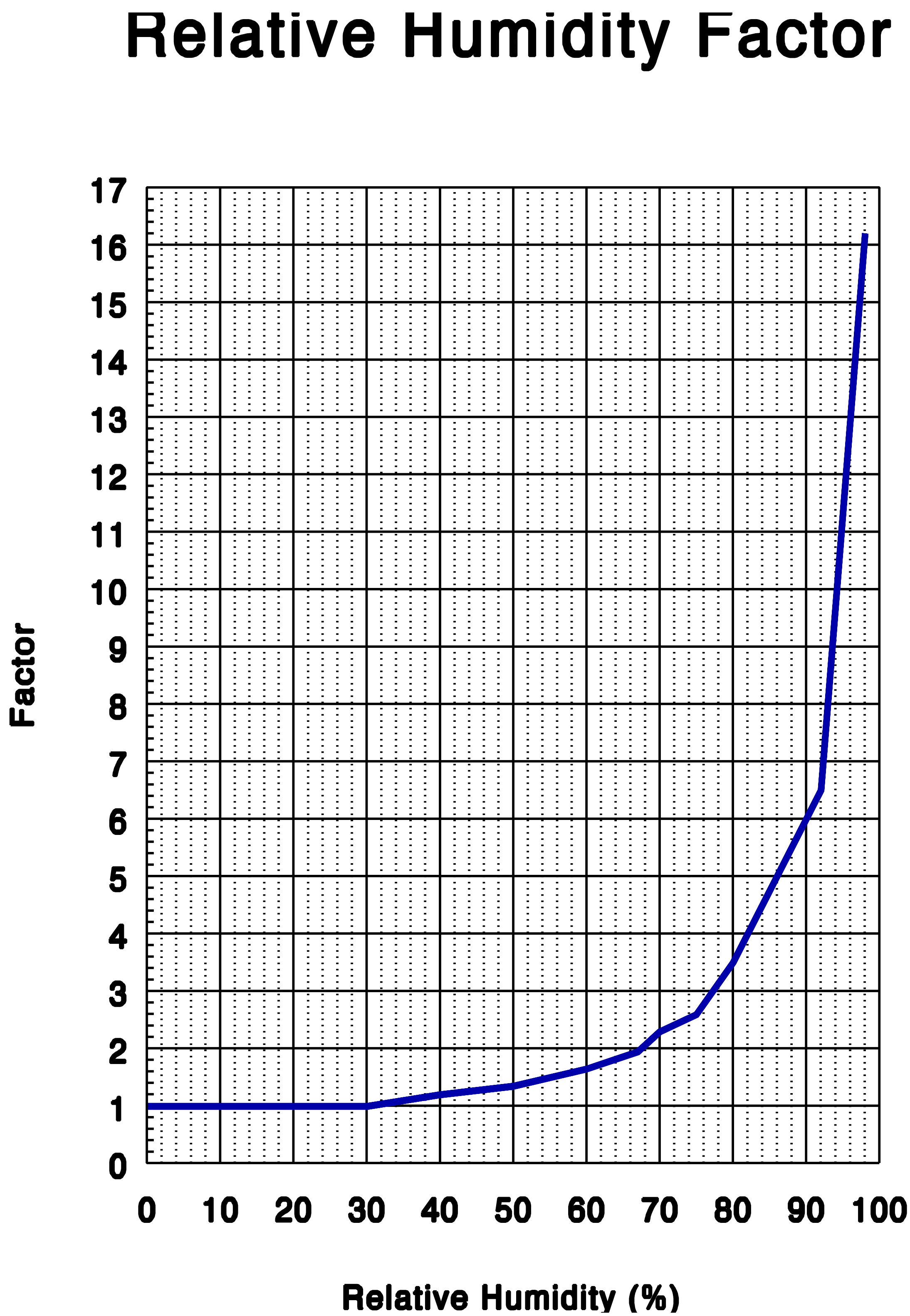

Figure B-1 - Correction factor to adjust for the effects of relative humidity on light extinction calculations (Tang *et al.*, 1981).

TABLE B-1. Relative humidity factor values versus humidity values used to construct Figure B-1.

Relative Humidity	Relative Humidity Factor
0.0	1
30	1
40	1.2
50	1.35
60	1.65
67	1.95
70	2.3
75	2.6
80	3.5
92	6.5
98	16

References

Tang, I.N., W.T. Wong, and H.R. Munkelwitz. 1981. The Relative Importance of Atmospheric Sulfates and Nitrates in Visibility Reduction. *Atmospheric Environment,* **15**(12):2463-2471.

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