Atmospheric Transport and Dispersion Modeling for the Hanford Environmental Dose Reconstruction Project

J. V. Ramsdell

July 1991

Prepared for the Technical Steering Panel

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Pacific Northwest Laboratory
Richland, Washington 99352

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This document has been reviewed
and approved by the Technical Steering Panel

John E. Till, Chairman
Technical Steering Panel
Hanford Environmental
Dose Reconstruction Project

July 2, 1991
Date

PREFACE

This report has two objectives. It 1) outlines the rationale used in selecting an atmospheric modeling approach for use in the Hanford Environmental Dose Reconstruction (HEDR) Project and 2) provides a brief description of the starting point for development of the atmospheric model used in Phase I of the project. Ramsdell and Burk (1991) provide a complete documentation of the MESOILT2 computer code used for atmospheric transport and diffusion calculations in Phase I.

This report was completed in draft form in the fall of 1989. The Phase I atmospheric transport calculations had been completed by the time the draft of this report was completed. An atmospheric transport workshop was convened in June 1990 to review the Phase I modeling approach. The invited workshop participants concurred with the modeling approach and suggested areas for model improvement. Phase I of the atmospheric modeling portion of the HEDR Project was completed in July 1990 with publication of the initial dose estimates.

Results of Phase I of the HEDR Project were analyzed during the following 6 months. This analysis led to the restructuring of the complete dose assessment methodology. The interface between the atmospheric transport model and the environmental model is one of the areas where major changes were required. Major changes were also required within the atmospheric model. These changes are associated primarily with the treatment of uncertainty in the meteorological and source term input to the model.

The atmospheric transport model is being revised at this time. The revisions will implement the changes required by the restructuring of the overall dose model and will include changes needed to improve the technical credibility of the model. When the atmospheric model revisions are complete, the model will be capable of generating sets of estimates of time-integrated air concentrations and surface contamination that are consistent with the input data and reflect the uncertainty in that data and in the atmospheric model. Model sensitivity will be examined following completion of model revisions, and the model will be evaluated using experimental data.

In light of the progress in the HEDR Project since the completion of the draft report, revisions to this report in preparation for final publication have been limited. No changes have been made to the appendices, and the changes to the body of the report have been primarily editorial.

Appendix F is a record of TSP comments and Battelle's response; the TSP has reviewed and approved these responses to their comments. Comment numbers appear in this report in the left margin next to the paragraph in which the corresponding comment was addressed. Changed text is shown italics. In addition to responses to TSP comments, some text was changed to correct errors or to provide clarification.

SUMMARY

The Hanford Environmental Dose Reconstruction (HEDR) Project has been established to estimate radiation doses people may have received from radionuclides released to the environment from operations that began at the Hanford Site in 1944. The project is being conducted by the Pacific Northwest Laboratory under the direction of an independent Technical Steering Panel. This report discusses the selection of an approach to estimating the transport and diffusion of radionuclides released to the atmosphere by operations at the Hanford Site for the HEDR Project.

A Lagrangian trajectory puff model has been selected as the primary method of estimating transport and diffusion. This type model uses available meteorological data to account for changes in atmospheric conditions as the radionuclides move away from the release point. These changes are important when concentrations of airborne radionuclides and surface contamination are estimated for locations that are more than a few miles from the release point. A straight-line model has been selected as a secondary model for estimating transport and diffusion near the release points. This type model is less complex because it doesn't account for changes in atmospheric conditions during transport. These selections are presented in the first section of the report. The first section of the report also discusses the modification of existing models to meet the project needs and evaluation of transport and diffusion models.

The second section of the report describes the various modeling alternatives that were considered. These alternatives, in order of increasing complexity, included box models, straight-line Gaussian models, Lagrangian puff models, gradient diffusion models, and particle-in-cell models. The report also presents information on the performance of various models. In general, increases in model complexity are accompanied by increases in time and cost. However, increasing model complexity beyond the Lagrangian puff models is not accompanied by a corresponding increase in model accuracy.

The final section of the report discusses additional factors considered in the selection of a modeling approach. These factors include the physical characteristics of the region in the vicinity of the Hanford site and the

meteorological data available for the region. The topography of the region and the distances between the release points on the Hanford Site and populated areas both suggest selection of an atmospheric modeling approach that accounts for temporal and spatial variations in meteorological conditions. Review of the meteorological data available for the region indicates that such an approach is feasible.

Five appendices present additional information related to the selected modeling approach. The first of these describes the MESOI model, which has been selected as the starting point for model development, and the next two appendices present evaluations of MESOI performance in two different applications. The fourth appendix contains a derivation of the family of straight-line Gaussian models. Finally, the last appendix describes six wind patterns that are common on the Hanford Site. These patterns further demonstrate why a modeling approach such as the Lagrangian puff model is needed in the HEDR Project.

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INTRODUCTION

Radiation doses that may have resulted from operations at the Hanford Site are being estimated in the Hanford Environmental Dose Reconstruction (HEDR) Project. One of the project subtasks, atmospheric transport, is responsible for estimating the transport, diffusion and deposition of radio-nuclides released to the atmosphere. This report discusses modeling transport and diffusion in the atmospheric pathway. It is divided into three major sections.

The first section of the report presents the atmospheric modeling approach selected following discussion with the Technical Steering Panel that directs the HEDR Project. The selected approach and the rationale used in the selection process are summarized. In addition, the section discusses the selection of the MESOI/MESORAD suite of atmospheric dispersion models that form the basis for initial calculations and future model development. Models to be used for the final atmospheric pathway calculations will be developed from the initial model set. A brief discussion of model evaluation ends the section.

The second section of the report describes alternative modeling approaches that were considered. It presents the alternatives in order of increasing complexity. Emphasis is placed on the family of plume and puff models that are based on Gaussian solution to the diffusion equations. The models in the recommended approach are members of this family. The final portion of the section describes the performance of various models. The models of the Gaussian family are shown to yield reasonable dispersion estimates over distances of several hundred kilometers. The expense of more complex models is shown to not be justified by an increase in model performance.

The third section of the report discusses factors that bear on the selection of an atmospheric transport modeling approach for HEDR. These factors, which include the physical setting of the Hanford Site and the available meteorological data, serve as constraints on model selection.

Five appendices are included in the report. Appendix A describes the MESOI dispersion model, which is the recommended starting point for model

development. Appendices B and C describe the performance of the MESOI model. The first of these covers the prediction of centerline concentrations and positions for individual plumes, and the other covers prediction of monthly average concentrations. Appendix D provides derivation of the family of straight-line Gaussian models. The basic equations for the Lagrangian puff model are developed as an intermediate step in derivation of the straight-line Gaussian models. Finally, Appendix E shows six common wind patterns for the Hanford Site. Three of these patterns, which occur a total of about 50% of the time, demonstrate directional variation in the wind fields. This variation is why a more complex model than a straight-line Gaussian model is needed for the HEDR Project.

ATMOSPHERIC TRANSPORT MODELING

Atmospheric transport modeling is an important aspect of the HEDR Project. Radionuclides have been released to the atmosphere from the Hanford Site during routine operations and in unplanned events. Atmospheric transport diffusion modeling is being used to estimate radionuclide concentrations in the air and surface contamination to supplement environmental monitoring data. This report documents the factors considered in selecting an atmospheric modeling approach.

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This section of the report is divided into three parts. The first part presents the selected modeling approach and a brief description of the rationale used in selecting a modeling approach. No existing model was entirely adequate for use in the project. *For example, no model computed the desired quantities, and no model addressed uncertainty.* Consequently, some model development work is required. The second part of this section suggests a starting point for model development and lists areas where model development may be required. The last part of this section suggests evaluation activities to establish uncertainties associated with the models being developed.

MODELING APPROACH

A 10-county region in Washington and Oregon has been selected as the domain for an initial phase of the HEDR project. These counties generally include the area within about 160 km (100 mi) of the 200 Areas at Hanford. Spatial and temporal variation in the atmosphere must be considered when evaluating transport and diffusion to these distances. Of the modeling approaches discussed in the next section, only the segmented plume, Lagrangian puff, gradient and particle-in-cell models have the flexibility needed to model transport and diffusion over the full HEDR domain. The straight-line Gaussian model is generally used near release points, but box models are not appropriate for any HEDR application.

A Lagrangian puff modeling approach has been selected for estimating air concentrations and surface contamination throughout the model domain, except near release points. This selection was based on a systematic elimination of

other alternatives. It is consistent with current practice in other programs dealing with atmospheric transport and dispersion to distances of a few hundred kilometers.

26,78 Studies of model performance *in experimental programs* indicate that gradient and particle-in-cell models require significantly more computational time than the simpler segmented plume and puff models without providing a corresponding increase in accuracy of transport and diffusion estimates. Considering that the source-term and meteorological data sets *available in the experimental programs* are more complete than the data sets available for the HEDR Project, the use of either a gradient or particle-in-cell model in the HEDR Project is unwarranted. Air concentrations and surface contamination estimated using the more complex models would be no more believable than concentrations and contamination estimated using the simpler models because the data would not support the more complex models.

71,89 The differences in performance between the segmented plume and Lagrangian puff models are largely a function of the algorithms and parameterizations selected by authors of the models. Although the times required to run the models for a month vary significantly, none of the model execution times poses a problem for the HEDR project. Choosing between a segmented plume and Lagrangian puff modeling approach involves a number of other considerations. These include general flexibility, availability of documented codes, and availability of alternative algorithms. In each case, the Lagrangian puff approach has the edge over the segmented plume approach.

A sector-average Gaussian plume modeling approach has been selected for use in estimating air concentrations and surface contaminations near release points. This approach was selected because atmospheric conditions and release rates may be assumed to persist during time required to transport material to the receptors within a few kilometers of radionuclide release points. A Lagrangian puff model could be used for this application. However, to do so would require a separate analysis using a finer resolution grid than is appropriate for the remainder of the HEDR domain. The data available for the periods of primary interest are not adequate to resolve small-scale spatial changes in meteorological conditions or short-term changes in release rates or

meteorological conditions. Consequently the simpler, sector-average Gaussian plume approach is the preferred modeling alternative for receptors near the source.

MODEL DEVELOPMENT

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The MESOI/MESORAD suite of models (Ramsdell et al. 1983; Scherpelz et al. 1986; Ramsdell et al. 1988) has been selected as a starting point for the development of the HEDR project atmospheric transport and diffusion models. This suite of models was developed for use in emergency response applications at Hanford. Appendix A contains a description of the MESOI code, which has been modified for use in climatological dispersion studies. The modifications are limited to data input and output; the transport and diffusion calculations are identical to those made in Version 2.0 of the code.

Some of the advantages of basing the HEDR models on the MESOI/MESORAD model suite are:

- The codes currently treat radioactive decay and wet and dry deposition. They also have modules that adjust wind fields for the anticipated effects of terrain. Consequently, the models can be used in their current state to estimate air concentrations and surface contamination in scoping studies.
- The current codes are highly modular. Descriptions of the processes involved in the transport, decay, diffusion and deposition of the radioactive material released during operations at Hanford can be modified easily, which will facilitate development of the HEDR codes.
- The performance of the current MESOI/MESORAD suite of codes is well documented. Thus, benchmarks exist that can be used to evaluate the effects of changes in the computational algorithms that are made as the HEDR models are developed. Appendix B presents an evaluation of MESOI predictions of plume centerline concentrations and plume positions using experimental data from the DOE Savannah River Plant. Similar results are obtained when the model is evaluated using experimental data from Hanford. Appendix C contains an evaluation of the performance of the modified version of MESOI in estimating monthly average concentrations.
- The models are fully documented and have widespread usage and can be assumed to be free of programming errors that would delay the development of the HEDR codes.

- The atmospheric sciences staff at PNL is familiar with the MESOI and MESORAD codes; no time will be lost while the staff learns new codes. In addition, the time required for debugging as the HEDR codes are developed will be minimized.

28.84 The current versions of the MESOI/MESORAD models were designed for use to distances of about 80 km (50 mi) with limited meteorological data availability off of the Hanford Site. As a result, all meteorological parameters vary as a function of time, but only the wind speed and direction vary as a function of position in the model domain. With the increased model domain in the HEDR project, the models should be modified to permit all meteorological parameters (*e.g., stability, mixing-layer thickness, and precipitation*) to vary spatially. Other areas where model development should be considered include

- iodine chemistry including conversion of I_2 to organic iodine and adsorption on particles
- deposition models including estimation of wet and dry deposition rates and depletion of deposited material from cloud
- improved representation of terrain effects on wind fields
- estimation of the mixing layer thickness
- estimation of the effects of plume rise and building wakes.

A sector-average, straight-line Gaussian model has been included in the MESORAD code for use near the release point. The code implementing the Lagrangian puff model provides a framework that includes meteorological data input for the straight-line code and many of the required computational modules. Portions of the code that require further development are the diffusion, deposition and depletion modules, and the model output module. These modules are much less complex in straight-line models than they are in puff models.

Specific model output will be determined by the needs of those making the dose estimates. For the initial phase of the study, time-integrated air concentrations ($Ci\text{-s}/m^3$) have been requested for all radionuclides, in addition, monthly average deposition rates ($Ci/m^2\text{-s}$) and the surface contamination (Ci/m^2) at the end of each month have been requested for depositing radionuclides. The atmospheric transport model will estimate these items at nodes

on a Cartesian grid. Post-processor programs will be used as necessary to convert the model output to any other form required for use in dose estimation.

MODEL EVALUATION

Model evaluation should be conducted concurrently with model development. This evaluation includes determination of the sensitivity of the concentration and contamination estimates to changes in data input and parameterizations of processes represented in the models and estimation of the uncertainty of the model estimates of the time-integrated air concentrations and surface contamination.

29.85 *Model* sensitivity to changes in parameterizations of the physical processes represented in the models should be evaluated. Specifically, model sensitivities to various *methods of calculating* plume rise, diffusion coefficients, and deposition need to be evaluated. In addition, the models' sensitivities to changes in the temporal resolution of the input data should be examined.

Uncertainty of the transport, diffusion, and deposition models should be evaluated by direct comparison of the monthly-average air concentrations and surface contamination predicted by the models with observed concentrations. These comparisons should be used to determine approximate distributions for the differences between model predictions and the observed values and to estimate parameters of the distributions. Temporal and spatial variations in the distributions and parameter values should be determined, if possible. Appendix C describes an initial effort along this line and describes additional data available for further model evaluation.

A lower-bound estimate of the uncertainty of the models should be evaluated using the best release and meteorological data available (probably the krypton-85 release and monitoring data for the years 1984 through 1986). The lower bounds should then be expanded to account for the additional uncertainty resulting from the limited meteorological and source term information available for the study period, as appropriate. These bounds will be appropriate for estimation of average air concentrations of nondepositing radionuclides.

Available monitoring data for depositing materials should be used to determine additional uncertainties associated with estimates of air concentrations and surface contamination for depositing radionuclides.

During the past year it has become clear that meteorological data records for the Pacific Northwest for the period between 1944 and 1948 are not as abundant as indicated in the National Climatic Data Center guides to available data. In addition, it has been determined that the Hanford Meteorological Station tower wind and temperature records for 1950 through 1952 are missing. As a result, secondary methods of estimating the meteorological conditions during periods with missing or sparse data should be examined. If reliable methods are identified, the meteorological data base will be expanded to include data that are needed for application of the methods.

ATMOSPHERIC MODELING ALTERNATIVES

This section of the report presents the range of modeling options considered. It includes a basic description of each type of model and a discussion of the performance of various models. Alternatives to modeling atmospheric transport and diffusion are covered in many texts and are the subject of continuing research. In general, the discussion proceeds from simple modeling approaches to complex. Detailed discussions of these approaches can be found in texts by Csanady (1973), Hanna et al. (1982), Pasquill and Smith (1983), and Randerson (1984). The section closes with a discussion of model performance.

BOX MODELS

Box models are the simplest method for estimating concentrations in the atmosphere. They have been used for regional, urban, and local air pollution studies where releases are distributed throughout the study area. They frequently assume that emissions are at ground-level and are uniformly distributed within the area, that the meteorological conditions are uniform throughout the box, and that there are no rapid changes in conditions (Hanna et al. 1982). In essence, a volume is defined, and material is assumed to be uniformly distributed throughout the volume. The amount of material may be adjusted to account for processes such as deposition and decay. The concentration is then estimated from its definition--mass divided by volume.

Box models have been used to study the temporal variation of concentrations in response to changes in source terms and meteorological conditions. However, Venkatram (1978) discusses the potential error in concentrations estimated by box models when the release rate decreases rapidly, and Hanna et al. (1982) more generally limit the application of box models to periods in which conditions change slowly.

Box models are based on an assumption that material is uniformly mixed; spatial variations of concentration cannot be modeled within a single box. Several adjacent boxes must be used if spatial variations in concentration are to be modeled. When this is done, material is moved from box to box using only the mean wind. Material does not move from one box to another as a

result of diffusion. Attempting to model small-scale spatial variations with box models results in extensive bookkeeping to maintain the mass balances that are needed for the concentration estimates.

Box models are inappropriate for use in the HEDR project for the following reasons.

- Releases to the atmosphere from operations at Hanford were generally from a few isolated release points rather than from area sources or a large number of release points distributed throughout the region. Assuming a uniform distribution of material within boxes of reasonable size will result in rapid "numerical" diffusion that is physically unrealistic and will tend to underestimate concentrations in the areas of most interest.
- Box models are not an efficient method for estimating the spatial distribution of the potential doses from Hanford operations. Other models are better suited to meeting that objective with no more complexity than required for a multiple-box box model.

PLUME AND PUFF MODELS

Gaussian models are a step above box models in complexity. These are the most widely used atmospheric transport and diffusion models. They describe the spatial variation of concentration in plumes explicitly. Appendix D outlines the derivation of the Gaussian models from the one-dimensional diffusion equation. Temporal variations in concentration may be estimated with a straight-line plume model by assuming a sequence of steady-state conditions, while segmented-plume and puff models use temporally varying input to model changes in concentration.

Although the models discussed in this section are referred to as Gaussian models, the concentration distributions generated by the models need not be Gaussian; the Gaussian label comes from the distribution assumed in the initial model derivation. Decidely non-Gaussian concentration distributions can result if diffusion is limited by boundaries or there are plumes from several sources.

Gaussian Plume Model

The Gaussian plume model is based on the assumptions that the conditions associated with transport and diffusion are constant in time and uniform in

space. If we establish a right-handed Cartesian coordinate system with the origin at ground level at or beneath the release point and orient the x-axis in the direction toward which the wind is blowing, the concentration in the plume at x,y,z is calculated as

$$C(x,y,z) = \int C \, dt$$

$$= \frac{Q'}{2\pi\sigma_y\sigma_z u} F(y) G(z) \quad (1)$$

where

C = concentration (mass/volume)

Q' = release rate (mass/time)

σ_y, σ_z = diffusion coefficients in the horizontal and vertical, respectively (length)

u = wind speed (length/time).

The diffusion coefficients are frequently referred to as the sigmas.

Significant effort has been expended in experimental determination diffusion coefficient values and in the development of algorithms for estimating them from more readily available information. Measurements of horizontal diffusion coefficients are relatively common, while measurements of vertical diffusion coefficients are rare. Draxler (1984) provides a summary description of the major diffusion experiments and their results.

Numerical algorithms used to estimate diffusion coefficients for regulatory purposes are based on data obtained within a few kilometers of the release point. In these algorithms, the diffusion coefficients are given as functions of atmospheric stability and distance from the release point. Other algorithms have been developed that give diffusion coefficients as functions of atmospheric turbulence levels rather than stability and time from release rather than distance. The use of time as a downwind variable rather than distance becomes more common as the distance of concern increase to 100 km (60 mi) and beyond (e.g., Hefter 1965, Gifford 1977, Draxler 1979, Draxler and Taylor 1982, Carhart et al. 1989).

The functions $F(y)$ and $G(z)$ describe the variation of concentration in the plume off of the plume axis. They are given by

$$F(y) = \exp\left[-\frac{1}{2}(y/\sigma_y)^2\right]$$

and

$$G(z) = \exp\left\{-\frac{1}{2}[(h - z)/\sigma_z]^2\right\}.$$

where

y = horizontal distance from the axis

h = effective height of release above the ground

z = distance above the ground.

As it stands, Equation (1) assumes that the earth's surface doesn't have an effect on diffusion. For most applications this assumption is not appropriate. The common means of accounting for the earth's surface is to assume that the surface reflects material reaching the surface. Reflection is incorporated in plume models by adding an imaginary second source of equal strength directly below the actual source at a height $-h$, which is beneath the earth's surface.

The net effect of addition of the imaginary source on Equation (1) is to change the definition of $G(z)$. The limiting effect of an inversion on vertical diffusion is incorporated in the model in a similar manner. Imaginary sources are added at various distances above the inversion and below the surface, with the result being an increase in the complexity of $G(z)$. Csanady (1973) provides a good description of the multiple reflections involved in modeling the effect of an inversion.

Long-term average concentrations and exposures (time-integrated concentrations) may also be estimated with a Gaussian plume model. However, the assumption implicit in Equation (1) that the meteorological conditions including wind direction remain constant is unacceptable when the time of release exceeds a few hours, and may even be wrong for shorter duration releases. As a result, a long-term, sector-average Gaussian model has been developed. In

the sector-average model, the concentration is assumed to be uniform across the plume. It is computed by first integrating Equation (1) from $y = -\infty$ to $y = \infty$ to obtain a crosswind-integrated concentration, CIC, and then dividing the CIC by the sector width.

If n is the total number of sectors into which the wind direction is divided, then the sector-average concentration, $C_{sa}(x,0)$ is

$$C_{sa}(x,0) = \frac{CIC}{\left(\frac{2\pi x}{n}\right)} \quad (2)$$

and the long-term average concentration at x in sector θ is

$$\langle C(j,x,0) \rangle = \sum_n \sum_s P(j,u,s) C_{sa}(x,0|u,s) \quad (3)$$

where

$\langle C(\theta,x,0) \rangle$ = the long-term exposure in sector θ at distance x and ground level

$P(\theta,u,s)$ = the joint probability of wind direction transport into sector θ , wind speed u and stability class s

$C_{sa}(x,0|u,s)$ = the sector average ground-level concentration at distance x , given wind speed u and stability class s .

The sector width is often determined by the resolution in wind directions. In recent years, in the United States wind directions have been recorded by 16 point compass headings (i.e., N, NNE, NE, ..., NNW) or to the closest 10°.

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The sector-average model implicitly assumes that the release rate is constant. As a practical matter, a less restrictive assumption that releases are random and independent of the wind direction, wind speed and atmospheric stability is adequate to justify the model.

It should be noted that the concentrations in these models are linearly related to Q . Therefore, as long as the assumption about release rates is acceptable, after a concentration is computed for one Q , concentrations for

other values of Q may be computed by simply scaling the initial value up or down.

The plume and climatological models just described are straight-line models. They assume that material, once released to the atmosphere, travels in a straight line indefinitely. They further assume that the atmospheric conditions everywhere and for the entire period of release are the same as the conditions at the time and location of release. Despite the limitations of these assumptions, straight-line Gaussian plume models are routinely used for diffusion estimates for environmental impact statements, for safety analysis reports, and for planning purposes. In each of these applications, the diffusion estimates are made for potential releases using assumed meteorological conditions. More sophisticated models are not used for these applications because all of the data entering into the diffusion estimates are predicted or assumed. Further, these estimates are generally made for the purpose of comparing one option with another. Straight-line models are also used routinely to evaluate the consequences of actual releases for regulatory purposes.

Segmented Plume Model

Segmented-plume models have been developed for use in applications where the assumptions of the straight-line Gaussian models are physically unrealistic. They follow directly from the straight-line model but include methods for treating temporal and spatial changes in atmospheric conditions. To treat the temporal and spatial changes in atmospheric conditions, these models separate dispersion into two parts, atmospheric transport, which determines where the plume is located, and diffusion, which determines the concentration at any location in the plume.

In a segmented-plume model, the plume axis is determined by a sequence of points emanating from the release at fixed intervals that mark the ends of plume segments. The transport portion of segmented-plume models move these points using winds estimated at the location of the points. The winds are determined as a function of time and location. Consequently, temporal and spatial variations in the winds are reflected in the plume location and shape.

14.30 Diffusion within plume segments is computed using a straight-line model
31 [Equation (1)]. Diffusion coefficients for each segment are determined using
the same parameterizations used in the straight-line models. The effects of
changes in atmospheric conditions along the plume trajectory are accounted for
by using different, imaginary release points for each plume segment. These
imaginary release points lie on extensions of the segment axes at distances
that are determined from the diffusion coefficients for the last time step and
the current meteorological conditions. In general there are two imaginary
release points for each segment; one for horizontal diffusion, and other for
vertical diffusion.

32 Segmented-plume models have been used for climatological dispersion esti-
mates. The computational requirements of these models make them more costly
than the straight-line model, but the costs are not prohibitive. The concen-
tration at a receptor at a specific time is determined by the sequence of
meteorological conditions between source and receptor for the time period
immediately prior to the time of interest. The time-integrated concentrations
are computed by summing the product of the concentration at each location and
the time-step interval over all time steps within the period of interest.

Both the temporal order of the meteorological conditions and the spatial
relationships in the meteorological conditions are important in determining
concentrations at a receptor. As a result, segmented plume models require
input of meteorological data as a time series rather than as a joint frequency
distribution. When meteorological data are available as a time series, dis-
persion estimates made with segmented-plume models should be better than
estimates made with straight-line models, because segmented-plume models use
information on temporal and spatial relationships that is not used in
straight-line models.

Lagrangian Puff Model

The segmented-plume model is more realistic than the straight-line model,
but it still has some problems. For example, the model is undefined when the
wind is calm, and estimation of concentrations near the ends of the segments
poses problems where there are bends in the plume. These problems can be
avoided by using a Lagrangian puff model. Lagrangian puff models are similar

to segmented-plume models in two respects. They separate dispersion into transport and diffusion components, and they track the position of the plume using points. The primary differences are in the interpretation of the meaning of a point, and in the model used to compute concentrations.

95,96 In a puff model, the points represent the centers of puffs rather than the endpoints of plume segments. There is no attempt to connect a point with other points released at different times. As a result, plumes are represented by disconnected *puffs*, and the *puffs* may move in different directions if the meteorological conditions are correct. Further, the concentration in vicinity of each point is computed using a puff model with appropriate boundary terms, and the concentration at each receptor is computed by summation of the contributions from all puffs.

Thus, the concentration at a position x, y, z in a puff not affected by physical boundaries is given by

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left\{ -\frac{1}{2} \left[\left(\frac{x - x_0}{\sigma_x} \right)^2 + \left(\frac{y - y_0}{\sigma_y} \right)^2 + \left(\frac{z - z_0}{\sigma_z} \right)^2 \right] \right\} \quad (4)$$

where the σ_x , σ_y , and σ_z are the longitudinal, lateral, and vertical diffusion coefficients and the center of the puff is at position x_0, y_0, z_0 . The diffusion coefficients are generally not equal, although σ_x and σ_y are frequently assumed to be equal.

97,98 Plume models are derived by integration of Equation (4). This integration is described in Appendix D. It is approximated in puff models by summation over all puffs at each receptor. This approximation can be made as accurately as desired by increasing the rate at which puffs are released and decreasing the time step. Ramsdell et al. (1983) show that if the ratios of the separation between puffs to the horizontal diffusion coefficient and of the distance moved in each time step to horizontal diffusion coefficient are less than two, the error in the approximation will not exceed 5%. Exposures are computed by multiplying the concentration by the time step.

Releasing four puffs an hour provides reasonable accuracy for emergency response applications of puff models. Reducing the release rate to two or

three puffs per hour may provide reasonable accuracy for climatological dispersion modeling of monthly exposures. Computing monthly exposures at each receptor is simply a matter of accumulating short-term exposures.

The computational requirements of puff models are larger than those of segmented plume models. This increase results from computation of the concentration in the vicinity of each puff and the summation over all puffs required to approximate the integral in Equation (4). However, the increase in computational load of the puff model relative to the segmented plume model is not matched by an increase in the overall total cost of the exposure estimates, because the cost is determined primarily by the preparation of the input data, and the models use the same input data.

A version of the MESOI puff model (Ramsdell et al. 1983) modified for use in climatological studies, requires less than 2 seconds computer time per hour modeled when the model is run on a VAX 11/780 computer. At this computation rate, it takes about 4 h to model transport and diffusion for a year.

GRADIENT DIFFUSION MODELS

Gradient (Eulerian) models form a third common approach to diffusion modeling. In these models the diffusion equation is solved numerically to estimate concentrations. The primary advantages of these models are that they are free of assumptions about concentration distributions and that they facilitate study of chemical processes in the atmosphere. They are particularly well suited to regional-scale modeling of diffusion from large area sources.

The three-dimensional diffusion equation that forms the starting point for these models is

$$\begin{aligned} \frac{\partial C}{\partial t} = S - \left(\frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial wC}{\partial z} \right) \\ + \left[\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial C}{\partial z} \right) \right] \end{aligned} \quad (5)$$

where

C = concentration at position x, y, z at time t

x, y, z = Cartesian coordinates

S = a source term that is non-zero only in the vicinity of the release point

u, v, w = transport velocity components in the x, y, z directions, respectively

K_x, K_y, K_z = diffusivities in the x, y, z directions, respectively.

The terms in the first set of brackets describe the rate of change of concentration resulting from advection, and the terms in the second set of brackets describe the change in concentration resulting from diffusion. Other forms of the equation treat diffusivity as a second-order tensor that results in additional diffusion terms. These terms are not shown because they may be assumed to be small in comparison with the terms shown (Hanna et al. 1982). Similarly, additional terms may be included in the equation to represent local sinks for mass. These terms have been neglected to be consistent with the discussion of other models.

Numerical solution of the diffusion equation involves integration of Equation (5) with appropriate initial and boundary conditions. Specification of boundary and initial conditions must be undertaken with care to ensure that they do not introduce artifacts into the solution that dominate the true solution.

33 The wind components and diffusivities may be specified as functions of time and position in model domain from available meteorological data. This requirement is similar to the data requirement for puff models. However, more care must be taken in specification of wind fields for use in gradient diffusion models. In puff models, the wind field affects only puff locations. In contrast, wind fields in gradient diffusion models affect both position and concentration. As a result, the wind fields for gradient models are fine-tuned to ensure conservation of the air mass.

34 The MATHEW code (Sherman 1978), which was developed at Lawrence Livermore National Laboratory to adjust wind fields for the ADPIC model discussed in the next section, is typical of the codes used to fine-tune the wind fields for

gradient diffusion models. Using a CDC-7600 computer, MATHEW requires several minutes to complete the adjustment process for a wind field defined at nodes of a 40 x 40 x 15 grid. The code also requires temporary storage of about seven times the number of nodes.

In addition to requiring better wind fields than puff models, gradient diffusion models require evaluation of concentration gradients at each location and each time step. If the concentration gradients are to be evaluated adequately, the spacing between nodes in the computational domain must be smaller than the characteristic dimensions of the plumes being modeled. Haltiner and Williams (1980) show that extremely large errors can occur in the estimates of derivatives as the spacing between nodes increases to one-half the characteristic size of a feature of interest in the field. The following example illustrates the effect of imposing this constraint on a gradient diffusion model.

Assuming that the characteristic width of a plume is six times the horizontal diffusion coefficient and that the spacing between nodes should be about one-third of maximum value gives an approximate spacing equal to the magnitude of the diffusion coefficient. If it is further assumed that the spacing should be able to resolve plumes during stable atmospheric conditions, then Table 1 shows the approximate node spacing needed to adequately estimate concentration gradients for a gradient diffusion model.

Even if the computational grid is sufficiently dense to permit computation of the gradients, the method of computing the gradients must be selected with care to avoid distortion and diffusion of the plume by the advection terms in the equation. Long and Pepper (1976) show the adverse effects of several numerical schemes used to solve the advection portion of the diffusion equation.

Numerical stability is also a concern in gradient diffusion models. The size of the time steps used in the numerical integration is limited by two stability criteria. One criterion is related to the advection terms, and the other to the diffusion terms. Haltiner and Williams give these criteria as $u \Delta t / \Delta x \leq 1$ for the advection terms and $2K \Delta t / \Delta x^2 \leq 1$ for the diffusion terms. In general, the criterion associated with the advection terms should be the

TABLE 1. Grid and Time Step Requirements for Gradient Diffusion Models to Resolve Concentration Gradients in a Plume and Maintain Numerical Stability

Distance (km)	Approximate Node Spacing		Associated Maximum Time Step (s)
	Horizontal (m)	Vertical (m)	
2	70	20	7
5	150	35	15
10	300	45	30
20	550	60	55
50	1300	80	120

more restrictive criterion. Using this criterion, the grid spacing required by stable atmospheric conditions and assuming a maximum wind speed of 10 m/s gives an estimate of the maximum permissible time step if numerical stability is to be maintained. Maximum time step estimates are included in the last column of the table.

As a result of the fine-tuning of the wind field, high grid density and small time steps, the computational requirements of gradient diffusion models are significantly greater than the segmented plume or puff models. Nested grids have been developed to minimize the computational load of gradient models while maintaining numerical stability. However, even with nested grids, the gradient diffusion models require larger computers and take longer to estimate concentrations than segmented plume and puff models.

PARTICLE-IN-CELL MODELS

Particle-in-cell models have been developed to retain the flexibility while eliminating some of the numerical difficulties of gradient diffusion model. They represent the diffusing material using particles. The position of each particle is tracked as the particles are advected and dispersed by the wind. The wind used for advection is a combination of an actual wind vector defined by a wind field model and a diffusive velocity vector defined by the diffusivity and concentration gradient. Concentrations are estimated counting

the number of particles in defined volumes (cells). Thus, the particle-in-cell models combine features of puff, gradient, and box models.

To adequately represent diffusion on the scales of interest, the number of particles and number of cells must be large. Lange (1978) describes the ADPIC model and gives several examples of its application. The basic model has 24,000 cells and can track 30,000 particles at any time. When used in its basic configuration, the model required about 90% of the large-core memory of a CDC-7600 computer and ran about 50 times faster than real time.

The MATHEW and ADPIC models are currently being run in combination on a VAX computer as a part of the Atmospheric Release Advisory Capability (ARAC) operated for the U.S. Department of Energy by the Lawrence Livermore National Laboratory. The computational time for the models has been decreased somewhat, but it requires a few minutes to compute the wind field and complete the diffusion computations for each hour. Assuming that the computations can be completed at the rate of 2 minutes per hour modeled, it would take approximately 12 days of computer time to complete computations for each year covered by the HEDR study using MATHEW and ADPIC.

Yamada and Bunker (1988) describe a model that combines the features of particle-in-cell and puff models. It tracks particles much as is done in particle-in-cell models, but it does not compute concentrations by counting particles. Rather, concentrations are computed by assuming that each particle represents the center of a puff and applying methods similar to puff models. This approach reduces the number of particles required while maintaining the flexibility of the particle-in-cell model. However, it still requires an accurate wind field.

MODEL PERFORMANCE

The preceding sections have described the classes of models that have been considered for use in the HEDR project. This section compares the performance of various models. It is based on model evaluations made using experimental data.

The results of the November 1980 model validation workshop hosted by the Savannah River Laboratory (Buckner 1981; Weber et al. 1982) are directly

applicable to the selection of models for HEDR. In preparation for the workshop, participants were provided hourly source-term and meteorological data for a 2-yr period and were asked to predict average concentrations at 13 locations between 25 and 150 km (15 and 100 mi) from the release point. Averaging periods for concentrations ranged from 10 h to 1 yr. The model predictions were then submitted to the Savannah River Laboratory for analysis. Table 2 shows a small subset of the results of that analysis.

Buckner (1981) describes each of the models. With one exception, the models listed as straight-line are sector-average models that used average release rates and meteorological data in the form of joint frequency distributions [Equation (3)]. The exception is the DRAX1 model. It is a sector average model that used hourly source-term and meteorological data. The trajectory models are equally divided between puff and segmented plume models; the first are puff models, and the last three are segmented-plume models. The last group of models includes models that involve numerical solutions to the diffusion equation [Equation (5)] and particle-in-cell models. MATHEW/ADPIC, PATRIC, and SRL-PIC models are particle-in-cell models, and the remaining models are gradient diffusion models.

The table lists estimates of the time required to predict monthly average concentrations and the computer for which the estimate is valid. This information is followed by Pearson correlation coefficients between predicted and measured concentrations for the model and the number of data pairs, in parentheses, used in estimating the correlation coefficient. The column headed R_m contains correlation coefficients for monthly average concentrations. The column headed R_w contains coefficients for weekly average concentrations, and the column headed R_{10} contains coefficients for 10-h average concentrations.

The salient points to be drawn from the table are related to the computational requirements of the various model types, the uses of the various model types, and the skills of the model types related to the concentration averaging interval.

The straight-line and trajectory models generally run on the same class of computer with the trajectory models taking about an order of magnitude

TABLE 2. Comparison of Atmospheric Dispersion Models Based on Savannah River Laboratory Analysis

Model	Time ^(a)	Computer	R_m ^(b)	R_w ^(c)	R_{10} ^(d)
<u>Straight-line</u>					
AIRDOSE-EPA	35	IBM 360	0.65 (155)		
XOQDOQ	20	IBM 360	0.56 (309)		
ATM	2	IBM ?	0.43 (335)		
DRAX1	20	IBM 360	0.42 (193)		
ANDEP	8	PDP 11/70	0.31 (348)		
<u>Trajectory Models</u>					
ASTRAP	190	IBM 360	0.75 (295)		
DRAGON GP	3.6×10^3	IBM 3033		0.51 (66)	
DRAX2	120	IBM 360		0.48 (419)	0.49 (381)
ATAD	1.2×10^3	IBM 360		0.48 (497)	0.21 (341)
DRAGON TH	600	IBM 3033		0.39 (66)	
ADPLUM	10^4	IBM 360		0.36 (258)	0.34 (273)
<u>Gradient Models</u>					
ATMOS1/ATMOS2	6.5×10^4	CDC 7600			0.80 (93)
MATHEW/ADPIC	10^5	CDC 7600			
PATRIC	4×10^3	CDC 7600			
SRL-CHAPEAU	1.63 ^(e)	IBM 360			0.64 (103)
SRL-MOMENTS	1.46 ^(e)	IBM 360			0.35 (103)
SRL-FOURIER	28.6 ^(e)	IBM 360			
SRL-PIC	1.0 ^(e)	IBM 360			0.25 (103)

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(a) Time in cpu seconds per month.

(b) Correlation coefficient between monthly concentration predictions and observations (number of points).

(c) Correlation coefficient between weekly concentration predictions and observations (number of points).

(d) Correlation coefficient between 10-hour concentration predictions and observations (number of points).

(e) Time relative to SRL-PIC.

longer to run. When the model complexity is increased to the gradient and particle-in-cell model level, the models are run on faster computers and the execution time increases significantly. In addition, once model complexity is increased to this level, the differences in computational time appear to depend more on the wind field characterization and the numerical schemes selected than on whether the model is a particle-in-cell model or a gradient diffusion model.

35, 74

The first two models in the third group are the only fully three-dimensional models. They take more than an order of magnitude longer to run than the trajectory models when run on larger and faster computers than used for the trajectory models. PATRIC takes about the same time as the trajectory models when run on the faster computer. The difference in execution speed between MATHEW/ADPIC and PATRIC is due to the time spent on preparation of the wind fields. Both models use three-dimensional wind fields, but the winds in the wind field used by PATRIC are constrained to be horizontal, while those in the wind field used by MATHEW/ADPIC are not. The SRL models have been included in the table, although the data provided in Buckner (1981) were not adequate to estimate run times, to provide additional information on the relative speeds of the particle-in-cell and gradient diffusion models. All of the SRL models use three-dimensional fields of horizontal winds. Thus, SRL-PIC, which is a particle-in-cell model, is approximately equivalent to PATRIC. The remaining SRL models are gradient diffusion models that use different numerical schemes to evaluate the concentration derivatives.

The Pearson correlation coefficients provide an indication of model skill in predicting the variations in the observed concentrations. The squares of these coefficients give the fraction of the variability in the observed concentrations that is accounted for by a model. In general, the coefficients increase with longer averaging times and increasing model complexity. However, the range in the correlation coefficients for each averaging period and the small number of models that predicted concentrations for more than one averaging interval make it difficult to estimate the improvement in skill in predicting monthly average concentrations that can be achieved by increasing model complexity.

Buckner (1981) and Weber et al. (1982) include comparisons of other indicators of model performance. Weber et al. conclude that the weekly concentrations were estimated about as well as the monthly concentrations. Ultimately, Buckner concluded that the more complex, three-dimensional models provide only marginal increases in accuracy over simpler codes when estimating monthly and weekly average concentrations, and that the cost of running the complex codes was not warranted for long-term releases.

More recent model validation and comparison estimates have focused on short-term concentration estimates and smaller distances related to emergency response applications of dispersion models. Eight models were evaluated in the second model evaluation workshop hosted by the Savannah River Laboratory (Weber and Garrett 1985; Weber and Kurzeja 1985; Kurzeja and Weber 1985). The object of the evaluation was prediction of concentrations 20 to 40 km (12 to 25 mi) downwind from 14 releases that were 15 minutes in duration. Six of the models evaluated were relatively standard puff models, one model was an advanced puff model in which puff dimensions were determined by a group of particles, and the last model was a particle-in-cell model. The ranking of the models depended on the statistical measure selected. However, it is clear from the analysis that the standard puff models can perform as well as the more complex models.

Model comparisons conducted for the U.S. Nuclear Regulatory Commission (Lewellen et al. 1985; Lewellen et al. 1987) using experimental data from Idaho and Wisconsin yield similar conclusions. The differences in the performance of simple and complex dispersion models are smaller than would be expected.

Recently Carhart et al. (1989) compared the performance of eight models in estimating concentrations at distances between 30 and 600 km (20 and 400 mi) from the release point in experiments conducted in Oklahoma and at the DOE Savannah River Plant. Of the models tested, two were segmented plume models, four were puff models, and two were more complex models. No one class of models performed significantly better than the others. Those differences that were noted were generally traced to differences in wind field representations and diffusion coefficient parameterization rather than to the model type.

ADDITIONAL MODEL SELECTION CONSIDERATIONS

Atmospheric dispersion modeling alternatives available for the HEDR Project have just been outlined. An atmospheric transport modeling approach could not be selected without considering both the physical characteristics of the northwest and Columbia Basin and the meteorological data available for input to the model. This information is presented here. The first part of the section describes the physical characteristics and the second the meteorological data.

PHYSICAL CHARACTERISTICS

A 10-county region of Washington and Oregon has been selected for the initial phase of the HEDR Project. These 10 counties include and border the Columbia River Basin. This description of physical characteristics covers the Columbia Basin topography and the population centers in and near the basin. It concludes by describing the atmospheric transport modeling domain selected to support the initial phase of the study.

Topography

Mountain ranges surround the Columbia River Basin and have a significant effect on atmospheric transport and diffusion in the HEDR study domain. There are also major hills and ridges within the domain that channel air flow, and under low wind speed conditions even the subtle topographic features on the Hanford Site are known to affect air flow.

Topographic features within the initial phase domain that affect atmospheric transport include: the Rattlesnake Hills, the Yakima and Umtanum Ridges, the Saddle Mountains, and the Horse Heaven Hills. These features deflect and channel the winds on the Hanford Site. They also form a basin in which air masses can stagnate. The Rattlesnake Hills, which follow the southwestern boundary of the Hanford Site and rise to an elevation of about 1000 m (3300 ft) msl, are particularly significant. They separate the Yakima River Valley from the Hanford Site and are responsible for some of the common features of the air flow over Hanford. Across the Columbia River from the Hanford operating areas is a series of bluffs that rise 100 to 200 m (330 to

660 ft) above the level of the river. These bluffs extend from the reactor areas almost to the Tri-Cities. Beyond the bluffs, the terrain to the east is characterized by rolling hills with a mean elevation that increases gradually.

Compared with the large scale topography, the topography of most of the Hanford Site is flat with small-scale features. It generally slopes toward the Columbia River near its eastern edge and to the southeast. The fuel processing facilities are located on the relatively level 200 Area plateau in the northwestern portion of the Hanford Site at a ground-level elevation of about 200 m (656 ft) msl. The edge of the plateau is defined by terrain sloping toward the Columbia River to the north, east, and southeast, and by terrain sloping into Cold Creek Valley from the south through west. Differences in elevation between the plateau and the adjacent lower ground are of the order of 50 m (160 ft), and the Columbia River is about another 50 m (160 ft) lower. As the Columbia River transits the Hanford Site, its elevation decreases from about 120 m (400 ft) to about 100 m (330 ft).

Other areas of interest on the Hanford Site include the reactor areas along the Columbia River on the north side of the Hanford Site, and the fuel fabrication facilities in the 300 Area near Richland. In these areas, the river and elevated terrain across the river are the most significant local topographic features affecting atmospheric transport and diffusion of effluents from these areas. In general, in each of these locations the prevailing winds tend to align themselves with the river.

The general features of the topography in the immediate vicinity of the Hanford Site are shown in Figure 1. The figure shows the current boundary of the Hanford Site, the operating area boundaries, smoothed elevation contours, and rivers. The 200 Area plateau and the 200 Areas are near the center of the figure. For reference, the center of the figure is 46° 30' N, 119° 30' W.

Population Centers

Although eastern Washington is generally sparsely populated, there are two relatively highly populated regions that are close to Hanford. The closest of these is the Tri-Cities Area on the southern border of the Hanford Site. It is about 40 km (25 mi) southeast of the fuel separations plants in the 200 Areas where most of the atmospheric releases took place. The other

FIGURE 1. Terrain of the Hanford Site and Surrounding Areas. The contour lines are labeled by single-digit numbers that represent elevation above sea level in hundreds of meters. Each contour line represents a change in elevation of 100 m (330 ft).

relatively highly populated region is the Yakima River Valley, between Yakima which is 80 km (50 mi) west of the fuels separations plants and the Tri-Cities. Both of these regions are within the domain for the initial phase study. Other population centers in the domain include Moses Lake, about 80 km (50 mi) to the north, and several small towns to the northeast and east including Othello and Connell, which are between 40 and 80 km (25 to 50 mi) from the fuel reprocessing plants. Spokane, which is the largest population center in eastern Washington, is about 200 km (125 mi) northeast of the Hanford Site.

Atmospheric Transport Model Domain

The irregular boundaries of the 10-county region which outline the domain for the initial phase of the HEDR project would be difficult to match in readily available atmospheric models because their domains generally have

rectangular boundaries. As an alternative to revising the structure of the model to permit irregular domain boundaries, a square atmospheric model domain has been selected that does not coincide exactly with the 10-county region. The domain, shown in Figure 2 extends west from Hanford to the Cascade Mountains, south to the Blue Mountains in Oregon and northeast to the Spokane area and includes the major population centers in the 10 county region. It is 256 km (160 mi) on a side and is centered at 46° 37' 30" north, 119° 00' west.

FIGURE 2. HEDR Phase I Study and Atmospheric Transport Modeling Domain

The MESOILT2 domain was offset from the 10-county area for three reasons. The first reason is that the prevailing wind patterns at Hanford have westerly components, which carry material released at Hanford to the east. Thus, offsetting the domain to the east increased the proportion of the domain that is downwind of Hanford in the prevailing atmospheric transport directions. The second reason is that winds with easterly components, which carry material to the west, are infrequent, are generally light, and do not persist for long periods. The third reason is that the terrain to the west of the MESOILT2 domain is mountainous. Concentration and deposition estimates for the western boundary of the MESOILT2 domain were assumed to be conservative estimates of the concentrations and deposition in the portion of the 10-county region to the west of the model domain.

METEOROLOGICAL DATA

Available meteorological data limit the accuracy of atmospheric transport. The meteorological data available for use in the study are described here. These data include extensive records for the Hanford Site and more limited records for the region. Wind patterns on the Hanford Site are also discussed. The section ends with a discussion of the adequacy of the temporal resolution of the data.

Hanford Data

Meteorological data for the Hanford Site are available from the records of the Hanford Meteorological Station (HMS). The first observations at the HMS, which is located on the 200 Area plateau between the 200-West and 200-East Areas, were made in December 1944. Since that time, with the exception of about a 2-1/2-yr period in the 1970s, the station has been manned on an around the clock basis. In the 2-1/2-yr period when it wasn't manned continuously, the station was manned on day and graveyard shifts. Wind and temperature data are available for all hours for this period because they were recorded automatically.

Data collected at the station include the standard surface weather observations and wind and temperature data from instruments mounted on a 122-m (400-ft) tower. These observations are made and recorded hourly. However,

the original data sheets for 1950, 1951, and 1952 are missing. Records for the observations from 1955 to date are available on magnetic media (e.g., magnetic tape and disks). Records of observations prior to 1955 existed as only as hand-written data sheets at the outset of the HEDR Project. These data are being entered into the Hanford data base.

Supplementary meteorological data have been collected on the Hanford Site during several periods. Of most interest are the supplementary wind data. At the present time there is a network of supplementary stations that provide wind and temperature data for 25 locations on and adjacent to the Hanford Site. This network, which is called the Hanford Telemetry System, is described by Glantz and Islam (1988). Complete data are available for Hanford Telemetry System starting January 1, 1982. Additional data are available for some of the locations beginning in the late 1970s. Summaries of wind data for early years of Hanford operations have been found for various locations on the Hanford Site. However, the summaries are generally not sufficiently detailed to be used as input to an atmospheric transport model, and further, the data on which the summaries are based are missing.

Regional Data Sources

The Hanford data provide a basis for estimating doses to the workers onsite, and perhaps to the general population near the site boundaries. However, meteorological data from the entire study area should be used when estimating transport to populations at larger distances. Indices to records stored at the National Climatic Data Center (NCDC) (e.g., Changery et al. 1977; Changery 1978; Hatch 1988) have been reviewed to identify the locations in Washington, northern Oregon, and northern Idaho for which meteorological records are readily available. These locations are shown in Figure 3. The stippled areas in the figure are mountainous and high regions. With a few exceptions, data are only available for locations in or near cities and towns along major interstate highways. As a result, the density of stations in eastern Washington and Oregon is relatively low.

The years for which records are available for each station within the period from 1944 through 1975 are shown in Figure 4. The most readily available of the records are those that have been digitized. These data generally

FIGURE 3. Pacific Northwest Locations with Meteorological Observations Between 1944 and 1975

contain hourly observations of current weather including wind speed and direction. Magnetic tapes containing the digitized data for many of the stations were obtained from the NCDC for previous research projects. Tapes containing the digitized data for the remaining locations have been obtained as part of the HEDR Project.

FIGURE 4. Available Meteorological Records for Pacific Northwest Locations, 1944 Through 1975

Figure 4 also shows periods for which undigitized data exist at the NCDC. Only periods with at least four weather observations per day are shown. When the observations were routinely made at scheduled times for use in preparation of weather maps, the data are listed as synoptic records. Otherwise, they are listed as hourly records. Hourly records may include 24 observations per day. Or they may include observations only during certain times; for example, observations may have been made only during daylight hours or when an airport was operating. Microfiche and photocopies of the original undigitized records have been obtained to supplement the digitized data. These data are being entered into the HEDR data base as needed.

Wind Patterns

Winds near ground level on the Hanford Site are affected by the local topography. Consequently, winds at an altitude of about 1500 m (5000 ft) have been used to determine long range transport patterns for effluents released at Hanford (e.g., Hilst 1951a, 1951b; Nickola 1951, 1952, 1953; Corley et al. 1977). In general, the patterns show a high probability of transport to the northeast, east and southeast.

Two analyses of surface level winds have been conducted as a part of the HEDR project. A version of the MESOI computer code (Ramsdell et al. 1983) was used to examine transport to distances of about 160 km using readily available data for 1964. The model results indicate predominant transport toward the northeast, which is consistent with the earlier analyses of winds at the 1500-m (5000-ft) level. In the other study, wind data from the Hanford Telemetry System for 1984 were examined using principal component analysis to identify common wind patterns (Skylingstad and Schwartz 1989). Details of this study are presented in Appendix E.

Six patterns have been identified and associated with the meteorological situations in which they typically occur. Five of the patterns are directly related to diurnal variations in the solar heating of the Columbia Basin. The other pattern, which is associated with strong weather systems, occurs at all times of the day with about equal frequency. Only three patterns, which occur less than 50% of the time, represent wind fields in which the winds are

relatively uniform throughout the Columbia Basin. The three remaining patterns, which occur more than 50% of the time, have a significant variation of winds across the Hanford Site.

A strong argument can be made for an atmospheric transport model that includes spatial and temporal variations of meteorological conditions on the basis of the frequency of occurrence of these three patterns. In one of these patterns the winds in the northwest portion of the Hanford Site are light and generally westerly while the winds in the southern portion of the Site are strong and southerly. This pattern, which is caused by diversion of the wind by Rattlesnake Mountain, occurs most frequently in the afternoon and evening. The other two patterns in this group occur most frequently at night and in the morning. One is a light wind drainage pattern in which winds flow toward the Cold Creek Valley at the base of Rattlesnake Mountain and toward the Columbia River and then generally flow to the south. In the remaining pattern, there are light to moderate southwest winds in southern and eastern portions of the Site, light to moderate northwest winds in the northern portion of the site, and the winds at the base of Rattlesnake Mountain are calm.

The meteorological data that are available for the model domain prior to the 1980s do not permit precise resolution of wind fields. Reporting stations are typically 50 to 75 km (30 to 50 mi) apart. As a result, the local wind patterns on the Hanford Site cannot be reproduced directly from the available data. However, it may be possible to infer the local wind patterns from available meteorological data including winds, pressures and temperatures.

Temporal Resolution

Typical times associated with radionuclide transport to receptors can be determined from the distance to the receptor and the average speed at the HMS, which is 3.4 m/s (Stone et al. 1983). Typical transport times to onsite workers are of the order of minutes (<1 h). Transport times from the fuel separation plants to offsite populations are of the order of a few hours rather than a few minutes. For example, 4 to 6 h would be required to transport effluents to the Tri-Cities. Transport times to Spokane or Portland would typically be of the order of a day--16 to 18 h for Spokane and 30 h for Portland.

For the onsite workers, the transport time is sufficiently short that the atmospheric conditions at the time of release can realistically be assumed to persist until the effluent arrives at the workers. Clearly, however, the time to transport effluents to major offsite populations is sufficiently long that it is unrealistic to assume that the atmospheric conditions at the time of release will persist from the time of release until arrival at these receptors. Meteorological data are generally available hourly. As a result, they will permit evaluation of the effect of changes in atmospheric conditions that occur between the time of release and time of arrival at distant receptors. Unfortunately, the temporal resolution in the meteorological data is likely to be better than the resolution in the source term data.

Staff members working on the Source Term Task indicate that the temporal resolution of the source-term information is variable. For some periods existing records may permit estimation of times of routine releases to within an hour or so. For other periods, routine releases are known to have followed systematic diurnal patterns but the times of individual releases are unknown, and some of the time there is little information that can be used to estimate the temporal characteristics of routine releases. Records associated with unplanned releases do not appear to contain sufficient information to permit estimation of the time of day of the release, and for many of these releases the information on when they occurred is no better than within a week, month, or quarter.

The effects of imprecise information on the temporal resolution of the releases are, to some extent, offset by the temporal resolution desired in the exposure estimates. Source terms for known releases occurring at undetermined times during a month can be combined and assumed to occur at a uniform release rate during the month. If there were a number of releases in this category and they occurred randomly throughout the month, the exposure and dose estimates should be usable. As the number and duration of the releases during the month decrease, the uncertainty associated with the exposure and dose estimates will increase.

While real plumes are well-defined entities that appear in photographs, atmospheric models describe plumes that represent conditions averaged over some finite period of time. The characteristics of plumes described by

atmospheric transport and diffusion models are a function of the averaging period as well as the atmospheric conditions during the period. For example, the apparent width of a plume increases as the length of the averaging period increases. This results because the plume changes position during the averaging period. Dose estimates in the initial phase of the HEDR project are to be made monthly. For periods of this length, plumes are only mechanisms used to estimate concentrations at points during the averaging period. The average concentration at any location for the period results from a series of events in which the plume is alternately present and not present. When the plume is present, the contribution to the average concentration is determined by the atmospheric conditions and distance to the release point. The frequency with which the plume is present is a function of direction and the wind pattern distribution.

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APPENDIX A

MESOI, AN INTERACTIVE ATMOSPHERIC DISPERSION
MODEL FOR EMERGENCY RESPONSE APPLICATIONS

PNL-SA-11669

APPENDIX A

MESOI, AN INTERACTIVE ATMOSPHERIC DISPERSION MODEL FOR EMERGENCY RESPONSE APPLICATIONS^(a)

PNL-SA-11669

J. V. Ramsdell
G. F. Athey
C. S. Glantz
Pacific Northwest Laboratory^(b)
Richland, Washington

ABSTRACT

MESOI is an interactive atmospheric dispersion model that has been developed for use by the U.S. Department of Energy and the U.S. Nuclear Regulatory Commission in responding to emergencies at nuclear facilities. MESOI uses both straight-line Gaussian plume and Lagrangian trajectory Gaussian puff models to estimate time-integrated ground-level air and surface concentrations. Puff trajectories are determined from temporally and spatially varying horizontal wind fields that are defined in three dimensions. Other processes treated in MESOI include dry deposition, wet deposition and radioactive decay.

INTRODUCTION

MESOI (Ramsdell, Athey and Glantz 1983) is an interactive atmospheric dispersion model developed for use by the U.S. Department of Energy, Richland Operations Office and the U.S. Nuclear Regulatory Commission (NRC), Office of Inspection and Enforcement for use in responding to emergencies at nuclear facilities. It has also been adapted for use by the Federal Emergency Management Agency in its Emergency Exercise Simulation Evaluation Facility. MESOI has its origins in the MESODIF Lagrangian puff model developed by Start

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and Wendell (1974). This paper describes MESOI and discusses some of the model's applications and limitations. A model, MESORAD, is being developed as an extension of MESOI to dose assessments.

There are several versions of MESOI. The latest version, which is described here, is intended for use on minicomputers that have virtual memories (e.g. the Digital Equipment VAX 11/700 and Data General MV-6000 and MV-8000 series computers). It requires approximately 200 kbytes of memory. However, by reducing the number and sizes of arrays in the model and by overlaying model segments, MESOI can be run on smaller computers. An earlier version of MESOI (Athey and Ramsdell 1982) is running in background on a small minicomputer.

BASIC MODEL FEATURES

MESOI combines Gaussian puff and plume models to estimate time-integrated ground-level air and surface concentrations of effluents released to the atmosphere. It accomodates multiple releases as defined by the user. The releases may occur serially or simultaneously from one or more elevated or ground level sources. If a source is a stack, the effective release height can be estimated using Briggs (1969) plume rise equations and the actual stack height.

A plume model is used to estimate the early contributions to concentrations at nodes on a polar receptor grid. The receptors are located at 10° intervals at nominal distances of 800, 1600, and 3200 m. These distances may be varied. For example, the distances on the inner arc could be set to the distances to the exclusion area boundary. Contributions to the concentrations at nodes on this grid from recirculating material are determined using the puff model.

Time-integrated concentration estimates, on a larger spatial scale, are accumulated at the nodes of a Cartesian grid. Spacing between the nodes is currently set at 2.5 km, but may be altered as required for a specific application. Only the puff model is used in accumulation of the concentrations on the Cartesian grid. Puffs are released at fixed intervals (nominally 15 min in current model applications) and moved in steps that are determined by the wind speed and puff dimensions. The minimum step interval is 1 min and the maximum is the interval between releases.

In addition to estimating time-integrated ground-level concentrations for nondepositing, nondecaying effluents, MESOI provides estimates of the surface contamination resulting from wet and dry deposition. It can also follow the decay of a radioactive effluent and the ingrowth and decay of a single daughter species.

Two sets of estimates are maintained for each grid. One set contains the time-integrated concentration estimates for the current release period (contributions from the current plume and all puffs) and the other set contains the accumulation since the start of the model simulation. Thus it is possible to use MESOI to approximate both current and long-term averages. The model also has an option that monitors long-term time-integrated concentrations at selected locations. If this option is exercised, an alarm is displayed when the time-integrated concentration at any of the locations exceeds predetermined values.

DESCRIPTION OF THE ATMOSPHERE

Puff dispersion models can make use of more comprehensive, and therefore, more realistic descriptions of the atmosphere than plume models. In MESOI, with the exception of the wind field, the atmosphere is defined as a single layer in which the properties (e.g. mixing layer depth, stability, temperature, and precipitation) are spatially uniform, but functions of time. Stability is defined as 1 of 7 classes, corresponding to the usual convention in which class 1 is extremely unstable and class 7 is extremely stable. Precipitation is categorized as liquid or frozen and each category is further classified by precipitation rate: light, moderate, or heavy. Extension of the model to incorporate spatial variation of these properties is straight-forward, but has not been done because data for input to the model are generally too limited to warrant it.

The MESOI wind field incorporates variations in both space and time. For purposes of defining the wind field, the atmosphere is divided into 3 layers: the surface layer, the layer above the top of the mixing layer, and the intermediate layer.

The surface layer (10 m) wind field is defined by interpolation and horizontal extrapolation of observed or forecast surface winds. The inverse

distance squared weighting scheme used in MESODIF, described by Wendell (1972), has been retained in MESOI. Goodin, McRae and Seinfeld (1979) indicate that this scheme provides a good compromise between accuracy and computational costs. In addition, MESOI has a provision for subjective modification of the surface wind field to account for effects of topography that may not be adequately represented in the wind observations or forecasts.

The top-layer wind is assumed to be uniform and representative for the entire model domain. While an observed upper-level wind may be used, other reasonable candidates include the gradient and geostrophic winds. These latter winds may be estimated from surface pressures or isopleths on weather charts. No provision is made for the adjustment of top-layer winds for topographic influences.

Winds in the intermediate layer are estimated by interpolating in the vertical between the surface- and top-layer winds at puff positions. Linear interpolation is used as a default. However, provision has been made for use of nonlinear interpolation if an appropriate scheme is developed. Interpolation is applied separately to the north-south and east-west wind components. As a result, both wind direction and wind speed shear are present in the intermediate layer.

The time variation of the wind field is treated by temporal interpolation of the surface- and top-layer fields between observation times.

The atmospheric conditions used by the plume model are derived from those used by the puff model. They are the conditions for the release point at the release time.

TRANSPORT

Explicit treatment of transport is an essential feature of puff models, and it is the separation of transport and diffusion that makes puff models more realistic than plume models. The movement of puffs is not constrained to any particular path based on winds at the release point and release time. Each puff moves in response to the wind vector at its current position. Effluent transport is not treated explicitly in plume models since their derivation generally includes an integration over the period of plume passage.

In MESOI, puffs move in response to the average of the winds linearly interpolated to the most recent and next puff release times. A puff transport vector is computed for the release period. Puff movement then occurs in shorter intervals that are subdivisions of the release period. These intervals are selected on the basis of puff dimensions and transport speed to permit reasonably accurate estimates of time-integrated concentrations while limiting the number of computations. The interval duration for the initial period is 1 min. As the puff grows, the intervals increase to a maximum value equal to the period between releases.

When a puff encounters terrain, its center of mass rises and falls as the terrain elevation directly beneath the center of mass rises and falls. Each puff is tracked until it leaves the Cartesian grid, or until the concentrations at its center falls below a minimum value.

DIFFUSION

Diffusion, in MESOI, is assumed to be Gaussian in the absence of boundary effects. The concentration distributions are functions of the horizontal and vertical diffusion coefficients, σ_y and σ_z , respectively. Horizontal cross sections through puffs are assumed to be circular, with a radius that is related to σ_y .

Four diffusion coefficient parameterizations are available for use with MESOI, although only one can be used at a time. These are: 1) the parameterization attributed to Eimutis and Konicek (1972) used in the NRC MESODIF-II, PAVAN and XOQDOQ models, 2) the "open country" parameterization (Briggs 1973), 3) the approximations to the Markee "desert" diffusion coefficients from MESODIF (Start and Wendell 1974), and 4) parameterizations recommended for use in urban areas (Ramsdell, Hanna and Cramer 1982). In each case, the diffusion coefficients are functions of atmospheric stability and distance from the source.

Vertical concentration distribution are Gaussian in the absence of boundaries; however, MESOI treats both the ground surface and the top of the mixing layer as reflecting boundaries. As a result, the vertical concentration distributions are not constrained to be Gaussian. When σ_z grows to 8/10 of the mixing layer thickness, MESOI assumes that the material is uniformly dis-

tributed in the vertical. If the effective release height is above the top of the mixing layer, MESOI treats the top of the mixing layer as a semi-permeable boundary, allowing material to descend through the boundary but not ascend through it.

DEPLETION

MESOI estimates the surface contamination from wet and dry deposition and depletes the airborne concentrations to account for deposition and radioactive decay of the effluent. If the initial effluent decays, airborne and surface concentrations of the daughter are estimated, with corrections for daughter decay if appropriate.

A source-depletion, dry-deposition model is incorporated in both the puff and plume models. In this model, a deposition velocity of 1 cm/sec is assumed in estimating surface contamination. Wet deposition is estimated using a washout model in which the washout coefficient is a function of precipitation type and rate. Following movement of a puff, the airborne material contained in the puff is corrected to account for deposition. The source term used with the plume model and close-in polar grid is not corrected for deposition.

The surface contaminations are intended only to indicate areas where high levels of contamination might occur, because the treatment of each of the deposition processes is rudimentary. It is expected that in the event of an actual release, quantitative information on surface contamination would be acquired as needed by monitoring teams.

MESOI permits three decay scenarios: a stable effluent that doesn't decay, an initial effluent that decays to a stable daughter, and an initial effluent that decays to an unstable daughter that decays in turn to a species that is of no interest. Both the initial effluent and the first daughter are followed. It is assumed that the daughter does not exist in the initial effluent.

MESOI does not estimate doses from the time-integrated air or surface concentrations. Dose estimates will be provided by the MESORAD model, which considers many radioactive isotopes simultaneously.

MODEL APPLICATION

MESOI is an interactive model that is intended for use in emergency response applications. The degree of interaction between the model and the user depends on the specific application. At Hanford, where there are many potential emergency scenarios and release locations, the interaction covers topics such as sources of meteorological data, grid dimensions, source locations and characteristics, release rate, release time and duration, and output options. For application at a nuclear power plant, the model can be tailored so that the interactions would be limited to release time and rate, and default values could be provided for these entries.

An emergency response model must provide timely output. Meteorological data files are used to minimize the delay between the time MESOI is started and the time output is available. At Hanford, the meteorological data files contain observations for the last 48 h and forecast data for up to 48 h. As a result, in the event of an emergency there is no time lost entering meteorological data. Initialization of the model takes about 2 min, and the first output is available a few seconds later.

Two plots, based on the surface wind data, are available. The first is a plot of the puff transport vectors at each of the wind observation locations. The transport vectors indicate the direction of puff movement and are the wind vectors rotated by 180° . The second plot contains the interpolated transport vectors at 5-km intervals on the Cartesian grid. These vectors include the effects of any subjective adjustments for terrain influence.

Puff positions and dimensions at the end of each hour can be written to a plot file. When plotted, the puffs appear as circles with radii that are equal to the distance from the puff center to a minimum concentration of interest. Puff positions are also indirectly indicated by the routines that monitor the time-integrated ground-level air concentrations at selected receptors. When the concentration rises above a predetermined level at one of the selected receptors, an alarm is displayed that gives the receptor location, the threshold and the time at which it was exceeded. At the end of a simulation, the status of the concentrations relative to the thresholds for all of the selected receptors is printed.

The final type output is a tabular presentation of the data for the nodes on each of the grids. If requested at the time of model execution, tables can be obtained for each release period, as well as cumulative tables for the entire simulation period.

MESOI LIMITATIONS

MESOI is a tool for use in evaluating the transport, diffusion and deposition of material released to the atmosphere. As with other tools, its use has limitations. MESOI's limitations generally fall in 3 areas: the relatively simple mathematical models used to approximate complex physical processes, the availability and accuracy of input data, and numerical compromises made to keep execution time and memory requirements within acceptable ranges.

The atmospheric processes in MESOI are represented by simple mathematical analogs such as the assumed Gaussian concentration distributions, the source-depletion dry-deposition model, the washout model, and the plume rise model. More complete representations of some of the processes are possible, but they require more data than is likely to be available on a routine basis. The programming structure of MESOI is highly modular to permit substitution of different mathematical analogs if desired.

Most of the models in MESOI describe average behavior. As a result, the concentration estimates produced by MESOI should be viewed as averages in a statistical sense. The estimates should not be expected to match observed values on a one-for-one basis for a specific set of atmospheric conditions. Concentration estimates for short duration releases are likely to be relatively inaccurate; the accuracy should improve as the release duration increases.

The concentration estimates of MESOI are sensitive to variations in input data. An uncertainty in the source term results in an equivalent uncertainty in the concentration estimates. Small uncertainties in estimates of effective release height or sigma z result in large uncertainties in concentration estimates near the source for elevated releases during stable atmospheric conditions. Uncertainties in the wind field are translated into uncertainties in plume and puff positions. As a result, concentration estimates for specific locations are less accurate than estimates of concentration as a function of

distance from the source because they include uncertainty associated with estimates of plume or puff position.

The numerical accuracy of the diffusion estimates of the puff model is a function of the number of times that a puff is sampled as it passes a receptor. Near the source where puffs are small, the estimates may be relatively inaccurate. There is also a reasonable likelihood that small puffs can move between relatively widely spaced receptors without being sampled, which would result in poor definition of the horizontal distribution of time-integrated concentrations. The plume model has been added to MESOI to makeup for these deficiencies in puff models.

SUMMARY

MESOI is an interactive atmospheric dispersion model for emergency response applications. Effluent transport is separated from diffusion and is estimated using Lagrangian trajectories in a 3-dimensional wind field. Gaussian puff and plume models are used to estimate diffusion. Surface contamination is estimated using a source depletion model for dry deposition and a washout model for wet deposition. The radioactive decay of a primary species and the ingrowth and decay of a single daughter are also treated.

MESOI is being used by the U.S. Department of Energy, the U.S. Nuclear Regulatory Commission and the Federal Emergency Management Agency. It runs on minicomputers and produces dispersion estimates within minutes of being started. An extension of MESOI, MESORAD, is being developed to produce dose estimates.

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APPENDIX B

COMPARISON OF MESOI ATMOSPHERIC DISPERSION ESTIMATES
WITH DATA AND ESTIMATES FROM OTHER MODELS
(PNL-SA-12670)

APPENDIX B

COMPARISON OF MESOI ATMOSPHERIC DISPERSION ESTIMATES WITH DATA AND ESTIMATES FROM OTHER MODELS(a) (PNL-SA-12670)

J. V. Ramsdell
C. S. Glantz
G. L. Andrews
Pacific Northwest Laboratory(b)
Richland, Washington

ABSTRACT

The magnitudes and positions of maximum short-term concentrations estimated by the MESOI and straight-line Gaussian dispersion models are compared with the magnitudes and positions of concentration maxima observed following 14 tracer releases at the DOE Savannah River Laboratory. Diffusion classes were selected using NRC temperature difference and sigma theta criteria.

The models' performances are compared statistically using analysis of variance and paired t-tests. The best performance is by the MESOI model using the split-sigma approach to selection of diffusion classes; the geometric mean ratio between the model's concentration predictions and the observed concentrations is 1.1. The split-sigma approach to selecting diffusion classes is found to be significantly better than the temperature difference approach.

INTRODUCTION

The MESOI dispersion model has been developed for emergency response applications by the Pacific Northwest Laboratory for the Richland Operations Office of the U.S. Department of Energy (DOE) and for the U.S. Nuclear Regulatory Commission (NRC) Office of Inspection and Enforcement. It is

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 - (b) Work Supported by the U.S. Department of Energy under Contract DE-AC06-76RLO 1830.

currently operational at the Hanford Site and in the NRC's Operations Center. We have evaluated the model in its operational form by comparing model estimates of short-term maximum SF₆ concentrations and their positions with the observed values contained in the Savannah River Laboratory (SRL) MATS data set. We have also made dispersion estimates with simpler straight-line trajectory Gaussian models to evaluate MESOI performance relative to the performance of alternative models.

The model results used in the evaluations and comparisons were obtained using initial estimates of atmospheric conditions (i.e., diffusion class and mixing layer thickness) made by a forecaster at Hanford. His estimates were based solely on the meteorological data contained on the MATS data tape. Although we have explored potential sources for differences between predicted and observed data, we have not included the results of any of the supplementary model runs in our evaluation. Our purpose in restricting ourselves in this manner is to evaluate the performance of the models as they would be used in an emergency.

MODEL DESCRIPTIONS

MESOI is a Lagrangian trajectory puff model that uses a Gaussian representation for the horizontal concentration distribution and a Gaussian representation with reflection terms for the vertical concentration profile within the puffs. The diffusion coefficients are computed as a function of distance traveled and atmospheric stability. Puffs are advected by the wind at the positions of their centers of mass. This wind is determined by horizontal, vertical, and temporal interpolation. The terrain was assumed to be flat for these dispersion computations. A complete description of MESOI is contained in Ramsdell, Athey and Glantz (1983).

Two modifications were made to MESOI to accommodate the MATS data set. The first was to change the reference height for the low-level wind field to 60 m from 10 m to account for the difference in wind measurement heights at the Hanford and Savannah River sites. The second change was to modify the MESOI code to permit it to compute concentrations at the specific receptor locations rather than at nodes on a fixed grid. Neither of these changes altered the computational algorithms in the code. A third alteration was

made to the code to permit evaluation of the split-sigma approach to selecting diffusion classes. In the split-sigma approach, the vertical diffusion class is determined by the temperature lapse rate and the horizontal diffusion class is determined by the standard deviation of the wind direction fluctuations. The operational version of MESOI uses the temperature lapse rate to determine the diffusion class for both vertical and horizontal diffusion.

MESOI was run in two modes. It was run in the normal mode in which the meteorological data are a function of time, and it was run using the release time meteorological data, assuming persistence. The first mode is the mode of operation used to follow the course of an event, while the second provides initial dispersion estimates. Assuming that short-term meteorological forecasts are reasonably accurate, evaluation of MESOI in these two modes should bound model uncertainty.

MESOI is small enough and fast enough to be run on small computers, but it cannot be run on hand-held calculators that may be used to provide a back-up or primary computational capability at some emergency response facilities. However, these devices can use straight-line trajectory Gaussian models to make diffusion estimates. Therefore, we made diffusion estimates using straight-line plume and puff models for comparison with the MESOI estimates. Meteorological data available at the beginning of the releases were used in the straight-line model computations.

With these model runs, we are in a position: 1) to compare the biases and uncertainties of the models, 2) to estimate the uncertainty in dispersion estimates that can be attributed to the use of persistence, and 3) to estimate the potential improvement in diffusion estimates that might result from the split sigma approach to estimating diffusion classes. Of course, these objectives can be met only within the limits of the experimental conditions.

DATA DESCRIPTION

The data used in evaluation and comparison of the models have been limited to the SRL MATS data sets. These data were obtained in 14 experiments that involved 15-min releases of SF₆ from a 62-m stack. The releases were distributed throughout 1983, although most (11) were in the second half of the year. All of the releases were made in mid-morning.

Samples were collected using sequential samplers located 20 to 40 km downwind of the release point. The positions of the samplers were selected prior to each release so that they would be spaced at about 1-km intervals across the expected SF₆ trajectory. The averaging time associated with the samples varied from 7 to 20 min, with most samples being 15-min averages.

Supporting meteorological data for the experiments include 60-m wind data from eight SRL towers and wind and temperature data from seven levels on a TV tower. The wind data include direction, speed, standard deviation of the direction fluctuations, and standard deviation of the fluctuations of the wind elevation angle. The data available at 15-min intervals were used.

The meteorological data files used by MESOI include the 60-m wind data, diffusion class specifications, and an estimate of the mixing layer thickness. Wind directions and speeds were rounded to the closest 10 degrees and 1 m/s respectively, because this would be required for use of the operational versions of MESOI. Diffusion classes were estimated using the criteria contained in NRC Regulatory Guide 1.23 (NRC 1974). The 37- and 93-m levels of the TV tower were used to determine the temperature lapse rate.

All model computations were made with meteorological data from the MESOI data files. The straight-line models and the MESOI persistence case were run with meteorological data available at the start of the release. Given the diffusion class or classes, the diffusion coefficients were computed using the "NRC" parameterizations described in the MESOI documentation. For all computations, the effective release height was assumed to be equal to the actual release height; plume rise was neglected.

The data used to compute the model comparison statistics were: 1) the maximum short-term concentrations for each MATS experiment and their effective transport directions and speeds estimated from the positions and time of the peak concentrations, 2) the same information derived from MESOI runs, 3) the center-line concentrations computed with the straight-line models for the distance to the maximum observed concentration, and 4) straight-line transport directions and speeds estimated from the wind at the H tower. Transport and diffusion are considered separately. The diffusion data used in the evaluation are listed in Table B.1, while the transport data are listed in Table B.2. There are two concentrations listed for each model in Table B.1. The first was

TABLE B.1. Maximum Short-Term SF₆ Concentrations (ppt). Concentrations under TD were estimated using diffusion classes determined by the temperature lapse rate, those listed under SS were estimated using the split-sigma approach.

Expt.	Obs.	Concentrations							
		MESOI		MESOI-Per		S-L Puff		S-L Plume	
		TD	SS	TD	SS	TD	SS	TD	SS
1	301.1	830.9	500.3	926.0	525.3	1240.9	1240.9	1208.0	1208.0
4	92.6	92.4	55.6	56.4	56.4	97.2	97.2	64.9	64.9
5	173.7	73.2	59.2	428.2	241.7	491.3	346.0	585.7	290.4
7	453.3	210.9	240.5	210.9	241.7	330.1	330.1	283.6	283.6
8	343.9	113.4	178.9	571.8	571.8	2098.0	2098.0	1028.2	1028.2
9	138.2	135.9	177.4	106.2	163.3	257.4	339.0	128.6	223.0
12	468.3	287.5	264.3	717.8	717.8	1098.8	1098.8	940.3	940.3
13	130.0	103.1	219.1	605.3	384.6	794.6	559.5	943.0	467.6
14	717.2	3137.2	1636.5	4791.1	2772.1	12202.8	8592.8	5656.5	2804.8
15	1112.2	2296.8	1402.8	2347.3	1400.7	3675.4	2588.1	3569.9	1770.1
16	196.2	3261.9	1358.9	4950.4	1371.8	6200.7	3104.8	5295.8	1327.0
17	151.8	879.5	509.0	1273.0	703.2	5673.2	2840.7	5136.6	1287.8
18	642.5	635.0	450.7	525.6	525.6	1142.0	1142.0	665.4	665.4
19	770.1	723.1	531.0	1804.0	1079.6	2245.9	1581.5	2731.3	1354.3

TABLE B.2. Effective Transport Directions and Speeds (km/hr)

Expt.	Transport Estimates (Dir/Spd)			
	Obs.	MESOI	MESOI-P	ST-Line
1	216.9/24.9	209.9/11.7	219.3/13.0	230/14.4
4	026.9/23.4	026.9/19.0	020.9/21.8	020/18.0
5	146.6/27.4	156.0/19.6	135.1/22.4	140/25.2
7	229.0/15.7	219.2/15.8	219.2/15.9	220/18.0
8	098.7/13.6	079.9/14.0	074.6/13.6	070/10.8
9	255.1/18.8	245.2/18.1	255.1/18.8	250/14.4
12	205.5/21.6	203.0/18.1	196.0/18.1	200/18.0
13	250.7/22.2	248.5/21.9	234.4/18.0	230/18.0
14	258.6/11.4	258.6/10.3	228.8/ 9.8	240/ 7.2
15	216.3/21.6	209.1/18.0	201.9/18.2	200/14.4
16	020.7/11.5	006.1/10.4	304.9/ 5.5	300/10.8
17	346.0/12.4	351.7/ 9.0	323.5/11.4	320/10.8
18	083.6/16.8	080.6/15.5	107.4/15.1	140/14.4
19	209.6/17.4	194.0/15.5	214.6/17.5	230/18.0

computed using a single diffusion class determined using the temperature lapse rate, and the second was computed with the diffusion classes determined using the split-sigma approach.

RESULTS

Historically, the results of diffusion models have been evaluated by enumerating the number or percent of the predicted concentrations within factors of 2 and 4, etc., of the observed values. Table B.3 provides a summary comparison of this sort for each of the four models and the two methods of selecting diffusion classes. A pair of numbers is given for each model and diffusion class selection method combination. The first number in each pair is the number of experiments where the ratio of the concentration estimated using the temperature lapse rate to the observed value is within the indicated range; the second number is for concentration estimates made using the split-sigma approach. From this summary it appears that model performance improves as you go down the list and that the use of the split-sigma approach to determining diffusion classes is better than only using the temperature lapse rate. However, comparisons of this sort are not readily amenable to statistical evaluation.

TABLE B.3. Summary of the Relative Errors in Maximum Short-Term Concentration Estimates of the Four Diffusion Models. The first number in each pair is the number of estimates for the 14 experiments within the range achieved using the diffusion class determined by temperature lapse rate (TD), and the second is the number when the split-sigma (SS) approach is used.

<u>Model</u>	<u>Relative Error</u>		
	<u>Factor of 2</u>	<u>Factor of 4</u>	<u>Order of Magnitude</u>
S-L Plume	4/4	8/8	11/11
S-L Puff	4/7	9/11	12/14
MESOI-Pers	5/10	10/12	13/14
MESOI	6/10	11/13	13/14

Use of the "factor of 2" type of comparison indicates that the magnitude of the ratio between the predicted and observed concentrations is a better indicator of model performance than is the difference between predicted and observed values. In the case of evaluation of diffusion models, the ratio is always positive and should be near one. As a result, the distribution of ratios is not likely to be normal, and statistical tests should not be applied directly to the ratios. However, use of a logarithmic transformation is likely to give an approximately normal distribution. (The logarithmic transformation is consistent with the use of log-log paper for plotting predicted and observed concentrations.)

Under these conditions, the appropriate measure of bias of a model is the geometric mean ratio between predicted and observed concentrations. Table B.4 compares biases of the four models using both of the methods of selecting diffusion classes. Again, the model performance increases as you go down the list and with the use of the split-sigma approach in selecting the diffusion classes.

The second column in Table B.4 gives correlation coefficients between the logarithms of the predicted and observed concentrations. These correlations are based on a linear regression of the log of the predicted concentration on the log of the observed. Had they been computed after forcing the regression

TABLE B.4. Comparison of Biases of the Four Diffusion Models and Correlations Between the Predicted and Observed Maximum Short-Term Concentrations. Biases are the geometric mean ratio between the predicted and observed values. Correlations are between the logarithms of the predicted and observed values. A bias and correlation is given for each of the methods of determining diffusion classes (TD/SS).

<u>Model</u>	<u>Bias</u>	<u>Correlation</u>
S-L Plume	4.18/3.41	0.49/0.57
S-L Puff	3.32/2.21	0.47/0.65
MESOI-Pers	2.29/1.67	0.53/0.68
MESOI	1.35/1.10	0.55/0.62

line through the origin, they would have been lower. In general, they indicate that there is a good deal of scatter in the data.

A two-way analysis of variance was conducted to establish the level of confidence that can be placed on the conclusions that can be qualitatively drawn from Tables B.3 and B.4. The results of this analysis are as follows: 1) there are significant differences (90% confidence level) between models, and 2) the differences due to the method of selecting diffusion classes are not highly significant (50 to 75% confidence level).

However, examining the results for the individual experiments reveals that the split-sigma approach improves model concentration estimates more frequently than it degrades them. A sign test shows that the difference in methods of selecting diffusion classes is highly significant (>99% confidence). Further, when the models missed the observed concentrations by more than a factor of two, the split-sigma approach improved the concentration estimates in almost all cases. In three of these cases where the concentration estimates were not improved, the estimates were unchanged. In the fourth case, the error in a MESOI estimate increased slightly but remained within a factor of four of the observed concentration. The degraded estimates generally occurred where the models did well when the temperature difference was used in selection of both diffusion coefficients. In these cases, the degradation was not large.

Contrasts between the means were conducted using Tukey's method for two-way comparisons and Scheffe's method for three- and four-way comparisons (Brownlee 1965) to determine which differences were significant. None of the differences between adjacent models were found to be significant (90% confidence level), i.e., the straight-line puff model was not better than the plume model, MESOI with persistence was not better than the puff model, etc. However, both MESOI models were better than the straight-line plume model, and MESOI with full data was better than either of the straight-line models. In addition, MESOI with full data was better than the average of all three models using only the meteorological data available at the start of release.

The biases and uncertainties of the effective transport vectors estimated with the models are compared in Table B.5. In this case, the data used for comparison are the arithmetic differences between predicted and observed transport directions and speeds. Given good model performance, the differences

TABLE B.5. Comparison of Effective Transport Estimates Made By the Straight-Line Models, MESOI with Persistence, and MESOI Using All Meteorological Data. Bias is the arithmetic mean error, and SD is the standard deviation of the errors. Direction units are degrees, and speed units are km/hr.

<u>Model</u>	<u>Direction</u>		<u>Speed</u>	
	<u>Bias</u>	<u>SD</u>	<u>Bias</u>	<u>SD</u>
Straight-line	-9.6	30.1	-2.8	2.5
MESOI-Pers	-13.5	22.6	-2.2	2.1
MESOI	-5.1	7.7	-2.2	2.3

should be approximately normally distributed about a mean of zero. One-way analysis of variance of the differences in effective transport directions indicates that models' performances are not significantly different. However, when paired differences are examined, the differences in transport directions are significant. The difference between MESOI with persistence and the straight-line models is significant at about the 90% confidence level, and the differences between MESOI with full data and the other models are significant at greater than the 95% confidence level.

DISCUSSION

The statistical analyses provide a limited view of the model performance. They address differences between models given the available data. They do not address the adequacy of the models for the intended applications, and they do not provide an evaluation of model performance in other meteorological conditions.

The MATS releases were made in a region of relatively simple terrain during mid-morning hours under meteorological conditions that, if not stationary, were at least predictable. These are the conditions under which a dispersion model should do well if it is to be useful in any condition. As a result, they are the conditions that are least likely to show the differences between models.

We would expect all of the concentration estimates made on the basis of meteorological conditions at the time of release to be biased to the high

side because the atmospheric stability is expected to decrease and the mixing layer thickness is expected to increase as the effluent is transported to the samplers. Both of these changes are associated with reduction in concentration. Further, the concentrations estimated by the straight-line Gaussian models should be high because of basic assumptions made in the models. Longitudinal diffusion is neglected in the plume model, but it is significant when transport times are much longer than the release times. Longitudinal diffusion is treated in the puff model, but the model estimates an instantaneous concentration at the center of the puff, which is higher than a short-term average during puff passage. The results are in conformance with these expectations.

The split-sigma approach to estimating diffusion classes clearly reduces the bias of the models and improves the correlation between the predicted and observed concentration estimates. Thus, the expected benefit of use of a physically more realistic method of selecting horizontal diffusion coefficients is borne out by these results. With respect to the selection of vertical diffusion coefficients, it is interesting to note that the case in which MESOI performed worst, Experiment 16, was the most stable case according to the vertical temperature profile. However, when the vertical profile of the standard deviation of the wind elevation angle is examined, it is obvious that the vertical diffusion should be good to at least 300 m. Blind adherence to the temperature difference criteria caused the vertical diffusion to be underestimated by at least two classes.

In the cases where the models' performances were worst, the mixing layer thicknesses at the time of release were estimated to be less than 250 m on the basis of the temperature profiles. In each case, the vertical profiles of the wind elevation angle standard deviation show that vertical diffusion is likely at and above the estimated top of the mixing layer. This clearly indicates that a better method for estimating mixing layer thickness should be established as a standard procedure for use with the models. Certainly, information on the vertical component of turbulence should be considered when available.

Our primary concern is the evaluation of dispersion models for use in emergency response applications. On the average, the diffusion estimates of

all of the models for these experiments are probably within an acceptable range. However, the performance of the models in several of the experiments (particularly Experiments 14, 16, and 17) indicates that their predictions can have significant errors. In these cases, the models overpredict the concentrations, which is desirable if they must be in error, but the errors may not always be overpredictions. Further, significant concentration overpredictions could lead to unnecessary actions that may be expensive.

The average error in MESOI transport direction estimates when all data were used was -5.4° with an average magnitude of 7.6° . When MESOI transport estimates were based on the meteorological data available at release time and a persistence assumption, the average direction error was -13.5° , and the average error magnitude was 18.0° . The transport direction errors of the straight-line models averaged -9.6° with an average magnitude of 22.4° . These averages are within a range that may be tolerable in selecting regions for protective actions in an emergency. However, the abilities of the models to make transport estimates were not severely tested by the range of experimental conditions.

The observed effective transport direction deviated by more than 30° from the transport direction estimated at the time of release in only two of the experiments, and by 20° in only six experiments. For these experiments, the average magnitudes of the errors in transport direction were 39° , 28° , and 10° respectively for the straight-line models, MESOI with persistence, and MESOI with full data. This comparison shows that potential errors are significant when release-time meteorological conditions are used to make transport direction estimates. It does not guarantee that errors made using full meteorological data will be small.

The transport speed estimates made by the models are lower than the observed transport speeds. This is to be expected on the basis of results of previous diffusion studies where the wind speeds at the height of release were used to estimate transport speed. However, it should be noted that average bias in the estimates is not much larger than the wind speed resolution in the MESOI input data, which is 1.8 km/hr. The uncertainty in the actual transport speeds is also about 2 km/hr when the typical wind speeds and durations of the sampling intervals are taken into account.

CONCLUSIONS

Short-term concentration estimates made with four dispersion models and two methods of selecting diffusion coefficients have been compared with observed data from the SRL MATS data set. The biases of the models ranged from a factor of 4.18 for a straight-line Gaussian plume model using diffusion classes selected on the basis of temperature lapse rate to a factor of 1.10 for MESOI using the split-sigma approach to selecting diffusion classes. Statistical analyses indicate that some of the differences between models are significant and that the split sigma approach to selecting diffusion coefficients significantly reduced the biases in concentration estimates.

Examination of the conditions under which the models performed worst indicates that the estimation of mixing layer thicknesses should receive more attention and that turbulence data should be considered, when available, in estimating mixing layer thicknesses and diffusion coefficients.

Transport estimates derived from the models were also compared with effective transport estimates derived from the data. The magnitudes of the MESOI transport direction errors were lower than the errors of the straight-line models, but there were no significant differences in the transport speed errors.

These conclusions are based on relatively few experiments conducted under a limited range of atmospheric conditions. The conditions were such that all models should perform well. As a result, the differences between models should be minimal. If similar data from experiments conducted under other, more severe, atmospheric conditions were to be analyzed, the performance of all models would be expected to be degraded, but the differences between the model should become more clear.

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APPENDIX C

ESTIMATION OF MONTHLY-AVERAGE CONCENTRATIONS
WITH THE MESOI DISPERSION MODEL

APPENDIX C

ESTIMATION OF MONTHLY-AVERAGE CONCENTRATIONS WITH THE MESOI DISPERSION MODEL

The performance of the MESOI model in estimating long-term average concentrations has been established by comparing model estimates of monthly-average concentrations of krypton-85 with environmental monitoring data at Hanford. This appendix describes evaluations of the MESOI model that have been completed to date. It describes the model's ability to estimate nominal monthly average concentrations and examines the sensitivity of model predictions to changes in diffusion coefficient parameterization, release height, and temporal resolution of the source term data.

INPUT DATA

The meteorological data base used in the prediction of average concentrations includes routine hourly surface weather observations, wind data for the 10-m level from a network of 24 stations, and wind and temperature data from towers. Glantz and Islam (1988) provides a comprehensive, up-to-date description of the meteorological data collection program for the Hanford Site.

The monitoring data used for comparison with the model predictions of the average concentrations consisted of individual samples of 14 to 38 days duration collected at six locations during 1984 and the first quarter of 1985. However, 51 of the 59 periods were between 27 and 30 days in duration. Table C.1 lists the names and locations of the monitoring stations and the number of samples for each station for which monthly and daily source-term estimates were available. The reported uncertainty (plus or minus two standard deviations) in the concentration estimates for individual samples due to counting error ranged from about 10 pCi/m³ for samples near background to between 10 and 15% for the higher observed concentrations.

TABLE C.1. Monitoring Locations and Available Data. The bearings and distances are from the PUREX plant stack.

<u>Location</u>	<u>Bearing (°)</u>	<u>Distance (km)</u>	<u>Samples</u>	
			<u>Source</u>	<u>Term</u>
			<u>Monthly</u>	<u>Daily</u>
Sage Hill	053	23.5	5	2
Ringold	089	22.9	15	1
Fir Road	119	25.4	9	3
300 Area	133	28.5	10	1
Prosser Barricade	152	19.2	8	3
Sunnyside	237	43.4	<u>12</u>	<u>2</u>
			59	12

STATISTICAL ANALYSIS

Linear regression was used to compare the predicted concentrations with the measured values. Historically, two different relationships between the predicted and measured concentrations have been assumed in evaluating atmospheric disperison models. The first relationship has the form

$$P = a + b M \quad (C.1)$$

where

P = the predicted concentration

M = the measured concentration

a, b = the regression coefficients.

The second relationship has the form

$$P = A M^d \quad (C.2)$$

where

P, M = the predicted and measured concentrations

A = 10^c

c, d = the regression coefficients.

This relationship may be linearized by making logarithmic transformations of the predicted and measured concentrations. When this is done, the regression coefficients may be determined using linear regression techniques. Atmospheric dispersion theory does not provide a basis for selecting one relationship over the other. It should be noted that the two relationships are identical under the following conditions

$$\begin{aligned} a &= 0 \\ d &= 1 \\ b &= 10c. \end{aligned}$$

The regression coefficients and the correlation coefficient provide an indication of model performance. Determination of the significance and confidence intervals for these coefficients is covered in statistical texts (e.g., Brownlee 1965 and Snedecor and Cochran 1980). If the dispersion model were perfect, the values of a and c would be zero, and b and d would have values of one. If the actual relationship is linear, the square of the correlation coefficient, which is commonly denoted as r^2 , is the fraction of the variation in the measured concentrations that is accounted for by the model. Values of r^2 near zero indicate that a model has little ability to predict the variations in concentration, while a value near one indicates a high level of predictability. Snedecor and Cochran (1980) contains procedures for evaluating and comparing correlation coefficients.

If values of r^2 alone are used to choose between the assumed relationships, the first relationship, i.e., the linear model given by (C.1) would be selected for use in model evaluation. However, linear regression techniques are based on the assumption that the variance of the dependent variable is a constant and not a function of the independent variable (see Brownlee 1965). The validity of this assumption can be evaluated by examining residuals from the regression where the residuals, R_i are defined as the differences between the dependent variables and the regression line, i.e.,

$$R_i = P_i - (a + b M_i). \quad (C.3)$$

Figures C.1 and C.2 show the residuals for the relationships indicated in Equations (C.1) and (C.2), respectively. Figure C.1 clearly shows that the scatter of the residuals for the linear model is a function of the independent

FIGURE C.1. Residual Errors for Linear Model as a Function of Observed Concentrations

FIGURE C.2. Residual Errors for Logarithmic Model as a Function of Observed Concentrations

variable. It is small for measured concentrations near zero and increases rapidly as the measured concentration increases. The scatter of the residuals for regression following logarithmic transformation of the variables (i.e., the logarithmic model) is a much weaker function of the independent variable, if it is a function of the independent variable at all. As a result, the model evaluation that follows is based on the transformed variables.

MODEL EVALUATION

The evaluation results are presented in tables that contain columns which describe the model or parameterization being evaluated and give the number of data pairs used in the regression, the estimates of the regression coefficients, standard errors of the coefficients, and r^2 . It should be noted that r^2 is not a particularly sensitive statistic for comparing models when there are few data points.

The results of comparing the observed concentrations with MESOI predictions of monthly-average concentrations for three sets of assumptions (cases) are shown in Table C.2. In the first case an 89 m release height is combined with the Nuclear Regulatory Commission (NRC) diffusion coefficient parameterization. This case matches the assumptions currently used in estimating atmospheric dispersion for the Environmental Monitoring Program annual reports. In the second case, the 89-m release height is changed to 61 m. This change ignores plume rise and yields slightly higher concentration estimates than the first case. In the third case, the 61-m release height assumption was retained, but the Desert diffusion coefficient parameterization (Ramsdell et al. 1983) replaced the NRC diffusion coefficient parameterization.

TABLE C.2. Regression Statistics for MESOI Based on Monthly-Average Source and Monitoring Data

<u>Release Height (m)</u>	<u>Diff. Coeffs.</u>	<u>n</u>	<u>c</u>	<u>s.e.</u>	<u>d</u>	<u>s.e.</u>	<u>r²</u>
89	NRC	59	0.0	0.368	1.170	0.025	0.583
61	NRC	59	0.0	0.423	1.214	0.028	0.540
61	Desert	59	0.0	0.419	1.190	0.028	0.538

The three cases yield essentially the same results. The model generally accounts for about 55 percent of the variability in the observed monthly mean concentrations. This performance is about the same as the performance of the best model in the Savannah River Laboratory model evaluation (Weber et al. 1982), and it is significantly better than the weighted average performance of all models used to estimate monthly mean concentrations.

The initial estimates of c were small compared to the standard errors of the estimates, and none of the values was significantly different from zero. Consequently, the regressions were redone assuming $c = 0$. Further, the values of d are slightly greater than 1.0 which indicates that the MESOI tends to overpredict the monthly average concentrations by a factor that increases with increasing concentrations.

Regression coefficient estimates can be used to correct model bias. Adjustment of the model concentration estimates involves rearranging the regression equation to solve for M given the MESOI prediction. M must now be interpreted as an improved estimate of the measured concentration rather than the measured concentration. To avoid confusion, M can be replaced by P' , where the prime indicated an adjusted model estimate.

Approximately 67% of the adjusted concentration predictions are within a factor of 2 of the measured values, and about 95% are within a factor of 4 of the measured values. The distribution of ratios between adjusted concentration predictions and the observed concentrations is approximately square-root normal. Neither normal nor log-normal distributions fit the data as well as the square-root normal distribution.

The ability of MESOI to estimate monthly-average concentrations at specific locations was examined by comparing the predicted and observed concentrations at each of the six monitoring locations during the 15-month period. Results of the site-specific comparisons are presented in Table C.3. The regressions for Sage Hill and Ringold are not significant. In the case of Sage Hill, the apparent lack of predictive ability is due, in part, to the small number of samples collected at that location. In the case of Ringold, the distance from the release point is relatively large and there are a

TABLE C.3. Regression Results for Individual Monitoring Locations

Monitoring Location	n	c	s.e.	d	s.e.	r ²
Sage Hill	5	1.904	0.327	0.092	0.349	0.023(a)
Ringold	15	1.389	0.292	0.485	0.262	0.209(a)
Fir Road	9	0.551	0.230	0.971	0.195	0.779
300 Area	10	0.710	0.237	0.911	0.231	0.661
Pros. Barr.	8	0.0	0.335	1.201	0.052	0.711
Sunnyside	12	0.0	0.182	0.947	0.033	0.705

(a) Not significant at the 90% confidence level.

sufficient number of samples to conclude that other factors are responsible for the lack of model's predictive ability.

The predictive ability of MESOI for monthly-average concentrations for the three monitoring locations near the southern boundary of the Hanford Site (Fir Road, 300 Area and Prosser Barricade) is greater than for the region as a whole. This may be due, in part, to the prevailing northwest winds in the 200 areas. The model's ability for the background monitoring location at Sunnyside is somewhat surprising, because the wind field adjustment scheme does not permit transport directly from the 200 East area to Sunnyside, and there are no meteorological data in the Yakima Valley.

The effect of improving source-term resolution on estimation of monthly-average concentrations was examined using Case 1 described in Table C.2 (NRC diffusion coefficient parameterization and an 89-m release height) with daily-average, source-term data for the first quarter of 1985. The results of the regression analyses are shown in Table C.4. Again, neither initial estimate of c was significantly different from zero, and the regressions were redone with c set equal to zero to get the results show in the table. The values of d may be assumed to be equal.

Improving source term temporal resolution to daily averages appears to improve the predictive ability of the model slightly. However, the significance of the difference in r² is limited by the small number periods with daily-average release data.

TABLE C.4. Variation of Regression Results MESOI for Monthly-Average Concentrations with Changes in Source-Term Time Resolution

<u>Temporal Res.</u>	<u>n</u>	<u>c</u>	<u>s.e.</u>	<u>d</u>	<u>s.e.</u>	<u>r²</u>
Daily	12	0.0	0.351	1.136	0.044	0.554
Monthly	12	0.0	0.352	1.166	0.044	0.592

Greater improvement in the model's predictive ability might have been expected to result from an approximately thirty-fold increase in source-term temporal resolution than is seen in Table C.4. An explanation for this result can be found by considering the nature of the releases. The model assumes that releases are continuous at a uniform rate until changed, but the process that releases krypton-85 is a batch operation in which the majority of the release occurs within a few hours of the beginning of the process. Thus, unless several batches of fuel are processed each day, the assumption of a continuous, uniform release can lead to errors in concentration predictions because the release is not properly correlated with the meteorological conditions.

The daily release data for the first quarter of 1985 indicate that about 50% time only one batch was processed per day. If processing generally started at approximately the same time of day on these days, the result could be a systematic error in model predictions. These systematic errors would occur because there atmospheric diffusion undergoes a well-developed diurnal cycle, and because there tends to be a systematic diurnal variation in wind flow patterns at Hanford. If the releases took place at night, assuming a continuous release would tend to result in the model underestimating concentrations. In contrast, assuming a continuous release will cause the model to overestimate concentrations if the releases tended to take place during the day.

FUTURE WORK

It is anticipated that model comparisons and model evaluations will continue as a part of the Hanford Dose Reconstruction Project. The data base used should be significantly improved over the current data base. The improvements in the data base will be made by increasing the period covered and by

obtaining better temporal resolution of the release periods. Extending the period used in model comparisons and evaluation to include the remainder of 1985 and all of 1986 results in a significant increase in the observations that can be used. Table C.5 shows the stations and number of periods for each station for which krypton-85 monitoring data are available between 1984 and 1986. There are a total of 214 concentration measurements in these three years, compared with the 59 measurements used in this study.

Not only are there more observations in the extended period, but the spatial distribution of the monitoring locations is also better in the extended data set than in the original. The locations of the monitoring stations used in this study are concentrated in the prevailing downwind direction. Monitoring stations added in 1986 provide a better regional distribution of locations. The only area of interest not covered by the 1986 monitoring stations is the area north of Hanford along the Columbia River.

Records exist that include the number of batches of fuel beginning the dissolution process each day. Records may also exist that permit determination of the shift on which each dissolution started. Thus, it should be possible to make future model comparisons and evaluations using source-term data with

TABLE C.5. Summary of Available ⁸⁵Kr Monitoring Data

Monitoring Location	Year			Total
	1984	1985	1986	
Othello	0	0	9	9
Sage Hill	2	12	12	26
Ringold	13	9	9	31
Fir Road	6	11	10	27
Eltopia	0	0	7	7
300 Area #1	9	10	11	30
300 Area #2	0	3	5	8
Pasco	0	0	13	13
Pros. Barr.	5	9	7	21
Sunnyside	9	12	11	32
Yakima	0	0	10	10
TOTAL	44	66	104	214

at least daily resolution. This potential improvement is further emphasized considering that there are only 12 measured concentrations in the original data set during the period for which there were daily source-terms.

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APPENDIX D

DERIVATION OF THE
STRAIGHT-LINE GAUSSIAN MODEL

APPENDIX D

DERIVATION OF THE STRAIGHT-LINE GAUSSIAN MODEL

The Gaussian models are of sufficient importance and utility that a derivation of several forms is outlined here. Derivation of the Gaussian models may be started with the equation for one-dimensional diffusion in a fluid at rest

$$\frac{\partial C}{\partial t} = K \frac{\partial^2 C}{\partial x^2} \quad (D.1)$$

where $\partial C/\partial t$ is the rate of change in concentration, K is the diffusivity, and $\partial C/\partial x$ is the derivative of concentration with respect to distance. If K is assumed to be a constant, then Equation (D.1) is the Fickian diffusion equation which for the boundary conditions

$$C \rightarrow 0 \text{ as } t \rightarrow \infty \text{ for all } x$$

$$C \rightarrow 0 \text{ as } t \rightarrow 0 \text{ for all } x, \text{ except } x = 0, \text{ and}$$

$$\int C \, dx = Q$$

where Q is the total mass being diffused has a solution

$$C = \frac{Q}{(4\pi Kt)^{1/2}} \exp\left(-\frac{x^2}{4Kt}\right) \quad (D.2)$$

where C is now a function of position and time. This equation has the form of a Gaussian distribution with variance

$$\sigma^2 = 2Kt$$

hence the name Gaussian diffusion model. It is common to refer to σ as the diffusion coefficient, or simply sigma. Significant effort has been expended in experimental determination of diffusion coefficients and in the development of algorithms for estimating them from more readily available information.

Assuming that diffusion proceeds independently in longitudinal, lateral and vertical directions, a solution to the three-dimensional diffusion equation can be obtained by superposition of solutions for the one-dimensional diffusion equation. Thus, the concentration at a position x, y, z in a puff not affected by physical boundaries is given by

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left\{ -\frac{1}{2} \left[\left(\frac{x - x_0}{\sigma_x} \right)^2 + \left(\frac{y - y_0}{\sigma_y} \right)^2 + \left(\frac{z - z_0}{\sigma_z} \right)^2 \right] \right\} \quad (D.3)$$

where the σ_x , σ_y , and σ_z are the longitudinal, lateral and vertical diffusion coefficients and the center of the puff is at position x_0, y_0, z_0 . The diffusion coefficients are generally not equal, although σ_x and σ_y are frequently assumed to be equal. Following Equation (D.3) the development of the common Gaussian plume and puff models takes different directions.

Gaussian Plume Model

Development of the plume model from this point requires a more refined definition of the coordinate system and location of the puff center than has provided. For convenience, the origin of the coordinate system will be assumed to be at ground level beneath the point of release. The positive x-axis is oriented in the direction of the movement of the puff (opposite the wind direction); the y-axis is perpendicular and to the left of the x-axis, and the z-axis is perpendicular to the x-y plane and pointed upward. Then, in this coordinate system, the center of the puff at any time following releases is given by

$$x_0 = u(t - t_0)$$

where u is the wind speed and t_0 is the time of release

$$y_0 = 0$$

$$z_0 = h$$

where h is the release height. The exposure (time-integrated concentration) at x, y, z is then

$$\begin{aligned} E(x, y, z) &= \int C \, dt \\ &= \frac{Q}{2\pi\sigma_y\sigma_z u} F(y) G(z) \end{aligned} \quad (D.4)$$

where

$$F(y) = \exp\left[-\frac{1}{2}(y/\sigma_y)^2\right]$$

and

$$G(z) = \exp\left\{-\frac{1}{2}[(h - z)/\sigma_z]^2\right\}.$$

The exposure in Equation (D.4) is still a function of distance because σ_y and σ_z are functions of distance (or time) and atmospheric stability.

For most applications it is not appropriate to ignore the potential effects of the earth's surface on vertical diffusion. The common means of accounting for the earth's surface is to assume that the surface reflects material reaching the surface. Reflection is incorporated in the plume model by adding an imaginary second source of equal strength at $0, 0, -h$, which is beneath the earth's surface. The exposure is then the sum of the contributions from the real and imaginary sources. Following completion of the algebra, the net effect of addition of the imaginary source on Equation (D.4) is to change the definition of $G(z)$. It becomes

$$G(z) = \exp\left\{-\frac{1}{2}\left[\frac{(h - z)}{\sigma_z}\right]^2\right\} + \exp\left\{-\frac{1}{2}\left[\frac{(-h - z)}{\sigma_z}\right]^2\right\}. \quad (D.5)$$

The limiting effect of an inversion on vertical diffusion is incorporated in the model in a similar manner. Imaginary sources are added at various distances above the inversion and below the surface, with the result being an

increase in the complexity of $G(z)$. Csanady (1973) provides a good description of the multiple reflections involved in modeling the effect of an inversion.

The standard Gaussian plume model is a special case of Equation (D.4) when $G(z)$ is defined by Equation (D.5) and $z = 0$. Then the exposure is

$$E(x, y, z) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp \left[-\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right] \exp \left[-\frac{1}{2} \left(\frac{h}{\sigma_z} \right)^2 \right]. \quad (D.6)$$

Equation (D.6) may also be used to estimate the average concentration during a period Δt if both the exposure and the mass are divided by Δt .

Frequently there is a need to estimate the long-term exposure or average concentration. Equation (D.6) involves an implicit assumption that the meteorological conditions including wind direction remain constant. This assumption is unacceptable when the time of release exceeds a few hours, and may even be wrong for shorter duration releases.

Equation (D.6) serves as the starting point for development of a climatological dispersion model based on the Gaussian plume model. A crosswind integrated exposure (CIE) is defined by

$$\begin{aligned} \text{CIE}(x, 0) &= \int E(x, y, 0) dy \\ &= \frac{2Q}{(2\pi)^{1/2} \sigma_z u} \exp \left[-\frac{1}{2} \left(\frac{h}{\sigma_z} \right)^2 \right] \end{aligned} \quad (D.7)$$

when $E(x, y, 0)$ is given by Equation (D.6). This crosswind integrated exposure is then redistributed over an angular sector to get a sector average exposure. The sector width is often determined by the resolution in wind directions. In recent years, in the United States wind directions have been recorded by 16 point compass headings (i.e., N, NNE, NE, ..., NNW) or to the closest 10° . If n is the total number of sectors into which the wind direction is divided, then the sector average exposure, $E_{sa}(x, 0)$ is

$$E_{sa}(x,0) = \frac{CIE}{\left(\frac{2\pi x}{n}\right)} \quad (D.8)$$

and the long-term exposure at x in sector θ is

$$\langle E(\theta, x, 0) \rangle = \sum_n \sum_s P(\theta, u, s) E_{sa}(x, 0 | u, s) \quad (D.9)$$

where

$\langle E(\theta, x, 0) \rangle$ = the long-term exposure in sector θ at distance x and ground level

$P(\theta, u, s)$ = the joint probability of wind direction transport into sector θ , wind speed u and stability class s

$E_{sa}(x, 0 | u, s)$ = the sector average ground-level exposure at distance x , given wind speed u and stability class s .

This model implicitly assumes that the release rate is constant. As a practical matter, a less restrictive assumption that the release rate is a random variable independent of the wind direction, wind speed and atmospheric stability is adequate to justify the model.

It should be noted that the exposures in these models are linearly related to Q . Therefore, as long as the assumption about release rates is acceptable, after an exposure is computed for one Q , exposures for other values of Q may be computed by simply scaling the initial value up or down.

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APPENDIX E

THE IDENTIFICATION OF TERRAIN-INDUCED
CIRCULATIONS USING PRINCIPAL COMPONENTS

PNL-SA-17164 HEDR

APPENDIX E

THE IDENTIFICATION OF TERRAIN-INDUCED CIRCULATIONS USING PRINCIPAL COMPONENTS PNL-SA-17164 HEDR^(a)

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E. D. Skillingstad and M. N. Schwartz

Pacific Northwest Laboratory
Richland, Washington

INTRODUCTION

The influence of terrain on local winds is a significant problem for air quality studies and forecasting for emergency response. Characterization of regional wind fields is usually accomplished using either wind roses or joint frequency tables of direction and speed. However, neither of these techniques provides a climatology of the wind field for an entire region. A technique providing both temporal and spatial wind field characteristics, or patterns, is needed to identify climatological winds throughout a region of variable terrain.

The method of multi-variate statistical analysis known as principal component (PC) analysis is of particular interest in identifying coherent patterns of wind direction. Both rotated and unrotated principal components have been routinely used to extract dominant flow characteristics from synoptic and large-scale meteorology (e.g., Kutzbach 1967; Horel 1981; Wolter 1989). The advantages of principal component decomposition include independence between the analyzed components (orthogonality), concise assignment of explained variance by each component, and the availability of robust statistical packages for performing the calculations.

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Here, both unrotated (PC) and rotated (RPC) principal components are used to identify complex terrain effects on the regional wind field patterns at the Hanford Site in south-central Washington State (Figure E.1). Hanford Site topography is dominated by the presence of two ridges in the west that define the Yakima River valley. The highest ridge, known as Rattlesnake Mountain, has a large influence on the site's meteorology, causing strong channeling and wake effects. On the larger scale, the Cascade Mountains to the west and the Rocky Mountains to the east generate a diurnal flow pattern prevalent in the warm season from April to October. By combining a knowledge of the synoptic meteorology of the Hanford Site with the wind patterns identified by the PC method, an interpretation of the terrain effects on the large-scale flow can be made.

PATTERN ANALYSIS TECHNIQUE

The primary goal of PC analysis is the reduction of large data sets to manageable scales. The PC method divides spatially and temporally dependent

FIGURE E.1. Columbia River Basin with Major Topographical and Geographical References. Contours represent elevation above sea-level in hundreds of meters.

data into patterns (the PCs) that explain the data variability with time-dependent scores and spatially dependent weightings. At any given time, the PC scores give a measure of the fit between the field of interest and the PC pattern corresponding to the score, and the weightings determine the importance of the station location in defining the PC pattern. In most cases, only three or four PCs are needed to explain the majority of the data variance. Therefore, the identification of the dominant PCs can lead to the construction of composite wind fields portraying the primary circulations within a region of complex terrain.

Mathematically, the PC model can be represented as

$$z_{nm} = \sum_{k=1}^K f_{nk} a_{km}^T$$

where z is an observed variable normalized to have zero mean and unit standard deviation with respect to time, f is the normalized PC score, a is the PC loading, $n=1, \dots, N$ represents an index in time, $m=1, \dots, M$ represents the station index, and k represents the PC number ordered by the portion of variance explained by the component (Richman 1986). In vector notation, the PC model is $Z = FA^T$.

Calculation of the PC loadings and scores is performed by computing a correlation or covariance matrix, solving for the eigenvalues and eigenfunctions (commonly referred to as Empirical Orthogonal Functions or EOFs) of the correlation matrix, and deriving the PC scores and loadings through simple matrix operations (see Richman 1986 for details). Rotation of the PCs is accomplished using the Varimax method (Cooley and Lohnes 1971), whereby the variance of the squared correlations between the time series of observations and the rotated PC is maximized. For a given RPC, this orthogonal transformation yields a more definitive weighing to some stations and reduces the importance of other observation locations.

The data analyzed consisted of 1164 4-hr averages of the wind components at 19 locations observed between 1/1/84 and 12/21/84. The number of 4-hr averages is less than the total possible because of the removal of those

periods with missing station winds. Each wind observation was standardized to unit speed to emphasize the directional influence of topography. From these data, a correlation matrix was generated along with the corresponding eigenvalues, eigenvectors and both PC and RPC loadings and scores. Each observation period was then assigned a dominant PC or RPC number (k) based on the maximum value of the component score, f_{nk} , for the three PCs and RPCs explaining the most variance in the data. Because each PC can describe two flow patterns, one opposite in direction to the other, the data were divided into a total of 12 different patterns. Cutoff PC scores of 1.25 and -1.25 were used to separate observations agreeing strongly with the PC modes from those not represented by the PCs.

Resultant winds were then calculated from these observations, giving a composite wind field for each PC and RPC pattern. A high PC score for a given observation frequently did not define a unique pattern when the variance explained by the PC was relatively small (i.e., PC numbers greater than 2). In addition, some of the resultant wind-field patterns did not differ significantly from another defined pattern, particularly between PCs and RPCs. Therefore, a subjective comparison of the composite wind fields to the individual component observations was performed to verify the existence and uniqueness of the resultant wind-field patterns. This approach reduced the number of significant patterns to eight flow situations corresponding to positive and negative PC 1, PC 2, PC 3 and RPC 1 (Figure E.2).

RESULTS AND DISCUSSION

In general, the patterns calculated using the above procedure represent the effects of topography combined with a particular synoptic large-scale flow situation. As an example, when weak southwesterly flow is dominant aloft, the typical local wind fields are represented by the pattern associated with positive PC 1. With this pattern, the flow is channeled through the Yakima Valley and around Rattlesnake Mountain, giving a cyclonic curvature to the wind field. Relatively weak winds are noticeable in the northern portion of the wind network with stronger winds near the Columbia River. In contrast, positive PC 2 demonstrates the effects of a strong southwest flow aloft with winds showing only minor local topographical obstruction.

Other features identified by the PC-derived patterns include the effects of diurnal heating and cooling. The positive PC 3 pattern is commonly observed at night with drainage winds converging on the river basin. On a larger scale, the wind-field pattern described by negative PC 2 is frequently witnessed during the afternoon when strong surface heating generates a thermal trough over the west side of the Columbia Basin with northeasterly flow over the Hanford Site. Another flow pattern forced by the regional topography is the well-documented Cascade drainage flow (Staley 1959; Stone et al. 1983;) represented by negative PC 1, showing strong northwest flow. The drainage flow pattern is often followed in early morning by the pattern associated with negative PC 3 as channeled southwest flow in the southern part of the Columbia Basin overcomes the northwest geostrophic forcing.

Because many of the flow patterns identified by the PC method appeared to reflect a diurnal heating and cooling cycle, the analysis effort was directed toward studying the interconnections and transitions between the patterns. For each observation period, the pattern with the maximum absolute score was determined. If the absolute maximum score exceeded 1.0, the observation was considered a member of the corresponding pattern. If the score fell below 1.0, the observation was classified as transitory. This information was used to determine a state-transition matrix, similar to a Markov process (Mo and Ghil 1988), whereby the probability of a given chain or pathway between patterns could be established. The maximum time allowed for a transition was set to 24 hours or 6 observation periods (i.e. a transitory state could not last longer than 1 day). Because many of the PC patterns displayed a high correlation with each other, only five patterns were considered for the transition matrix, all from unrotated PCs (Table E.1).

An interpretation of the transition matrix in Table E.1 is possible for the high-frequency changes (shown as underlined values). The high probability of transition from negative PC 1 to positive PC 2 demonstrates the typical changes that follow the occurrence of a strong Cascade drainage event.

Positive Principal Component 1

Positive Principal Component 2

FIGURE E.2. Wind Vector Plots of Dominant Principal Components Calculated from 4-hr Average Winds from 1984 at the Hanford Site Wind Network

Positive Principal Component 3

Negative Principal Component 1

FIGURE E.2. (contd)

Negative Principal Component 2

Negative Principal Component 3

FIGURE E.2. (contd)

Positive Rotated Principal Component 1

Negative Rotated Principal Component 1

FIGURE E.2. (contd)

Further evidence of this pattern sequence is provided by a frequency table for the patterns as a function of averaging period (Table E.2), which demonstrates an increase in occurrence of positive PC 2 during the morning as the Cascade drainage circulation decreases. The transition from positive PC 3 to negative PC 2 is commonly observed during summer months and is in response to a thermal trough in the Columbia Basin with a surface high over southern Alberta, Canada without the Cascade drainage circulation. Other high-frequency transitions noted in Table E.1 can be attributed to either the daily drainage cycle or the effects of increased mixing in the afternoon period (e.g., positive PC 1 to positive PC 2).

CONCLUSIONS

The application of principal component analysis to regional wind fields can provide an objective method for the identification of synoptic, thermal, and topographical effects. These results can be applied to regional wind forecasting by providing a frequency distribution for various wind-field transitions from the current observed state or used in defining climatological wind fields for air quality studies. In future work, a principal component analysis of large-scale forcing will be combined with the regional wind-field study to provide a more objective link between synoptic and mesoscale patterns. Synoptic-scale situations from operational meteorological models could then be used to predict changes in the local wind field.

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TABLE E.1. Transition Matrix for the Three Principal Components from the Wind-Field Analysis with the Average Persistence for Each Pattern. The column principal component is the initial state with the row representing the final state. Observation times without a PC score greater than 1.0 were recorded as a transition pattern.

Persistence: (Hours)	Initial State				
	PC+ 1	PC- 1	PC+ 2	PC- 2	PC+ 3
	7.2	9.5	7.0	7.5	7.2
PC+ 1	20	24	<u>29</u>	12	25
PC- 1	20	14	<u>33</u>	<u>28</u>	16
PC+ 2	<u>31</u>	<u>38</u>	8	2	5
PC- 2	14	22	5	0	<u>27</u>
PC+ 3	<u>26</u>	14	10	<u>25</u>	4

TABLE E.2. Principal Component Occurrences as a Function of the 4-hr Averaging Period. Observations were limited to those with absolute PC scores greater than 0.5.

Pattern	Hours of Occurrence					
	24 - 4	4 - 8	8 - 12	12 - 16	16 - 20	20 - 24
PC+ 1	12	23	21	47	50	36
PC- 1	65	23	19	11	20	65
PC+ 2	29	36	27	35	41	27
PC- 2	5	10	18	28	46	15
PC+ 3	47	40	18	0	4	24
PC- 3	60	75	77	41	29	40

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transformation of the three principal components from the principal component analysis. The first component is the one with the largest variance, the second component is the one with the next largest variance, and the third component is the one with the next largest variance. The three principal components are uncorrelated and their variances are equal to the eigenvalues of the covariance matrix of the three principal components.

Principal Component Analysis			
Component	1	2	3
1	0.70	0.25	0.05
2	0.25	0.70	0.05
3	0.05	0.05	0.70
4	0.05	0.05	0.05
5	0.05	0.05	0.05
6	0.05	0.05	0.05
7	0.05	0.05	0.05
8	0.05	0.05	0.05
9	0.05	0.05	0.05
10	0.05	0.05	0.05

Figure 1. Principal component analysis of the three principal components. The first component is the one with the largest variance, the second component is the one with the next largest variance, and the third component is the one with the next largest variance. The three principal components are uncorrelated and their variances are equal to the eigenvalues of the covariance matrix of the three principal components.

Principal Component Analysis			
Component	1	2	3
1	0.70	0.25	0.05
2	0.25	0.70	0.05
3	0.05	0.05	0.70
4	0.05	0.05	0.05
5	0.05	0.05	0.05
6	0.05	0.05	0.05
7	0.05	0.05	0.05
8	0.05	0.05	0.05
9	0.05	0.05	0.05
10	0.05	0.05	0.05

Figure 1. Principal component analysis of the three principal components. The first component is the one with the largest variance, the second component is the one with the next largest variance, and the third component is the one with the next largest variance. The three principal components are uncorrelated and their variances are equal to the eigenvalues of the covariance matrix of the three principal components.

Figure 1. Principal component analysis of the three principal components. The first component is the one with the largest variance, the second component is the one with the next largest variance, and the third component is the one with the next largest variance. The three principal components are uncorrelated and their variances are equal to the eigenvalues of the covariance matrix of the three principal components.

Figure 1. Principal component analysis of the three principal components. The first component is the one with the largest variance, the second component is the one with the next largest variance, and the third component is the one with the next largest variance. The three principal components are uncorrelated and their variances are equal to the eigenvalues of the covariance matrix of the three principal components.

APPENDIX F

SUMMARY OF TSP COMMENTS AND BATTELLE RESPONSES

SUMMARY OF TSP COMMENTS AND BATTELLE RESPONSES

Document Number PNL-7198 HEDRDocument Title Atmospheric Transport and Dispersion Modeling for the Hanford Environmental Dose Reconstruction Project

Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
1.	David Price		Coverage of forecast evaluation and principal components in Appendixes B, C, E would not meet the standards of the economics profession.	Appendixes B, C, and E were written for other purposes. They have been included in this report because they may provide information of interest to some members of the TSP and the public. These appendixes have not been revised because they represent completed work. Future statistical analyses will be performed with the assistance of project statisticians using appropriate techniques.
2.	DP		The forecast evaluation techniques are generally outdated and do not highlight the weaknesses of the forecasts.	See response to comment 1.
3.	DP		The r value between the measured values and the predicted values fails to measure any systematic bias in the forecast.	See response to comment 1.
4.	DP		The technique of regressing the increased and predicted values of the slope and intercept to 1 and 0, respectively, has been criticized by Granger and Newbold.	See response to comment 1.
5.	DP		Selection of functional form for the forecast evaluation regression. Authors selected log-log form to avoid heteroscedasticity; economists select the functional form on the basis of the form of the relationship.	See response to comment 1.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
6.	DP	Page C.3, last paragraph	The correct assumption of the general linear model is that the variance of the error term is constant.	Correct.
7.	DP	Page E.3	Should provide a term expressing the variance specific to each variable, define the PC's, and present the criteria used to extract the components.	This appendix is a paper presented at a poster session. The appendix was included to illustrate common wind field patterns near Hanford, not to describe application of principal component analysis to vector fields.
8.	DP		The values of the eigenvalues need to be presented.	See response to comment 1.
9.	DP		A complete discussion of the selection of the number of PC's used is needed, so this decision does not appear purely subjective.	See response to comment 1.
10.	DP		The report presents both rotated and unrotated PC's. A clear discussion is needed of the characteristics of each.	See response to comment 1.
11.	Bernard Shleien		The report provides no information of substance as to preliminary results. Should give actual data on parameters specific to Phase I, and uncertainties associated with the models used.	This report documents the rationale for selection of an atmospheric modeling approach.
12.	BS		The report states: "The statistical analyses provide a limited view of the model performance" It is inappropriate to present data only on statistical analysis.	See response to comment 1.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
13.	BS		Without some information on the uncertainties, or the variance that could be expected due to specific decision points, one cannot judge the utility of the results for Phase I.	See PNL-7340 HEDR and PNL-7199 HEDR for assumptions related to uncertainty in MESOILT2. Uncertainty will be addressed in detail in the revised atmospheric model.
14.	D. S. Barth	Page 14	Lines 3 and 4 from the bottom of the page. Change this to whatever was intended.	Deleted extra words.
15.	DSB		Add section describing how variances or possible errors in estimated values will be quantitated for the model and input data (required for uncertainty analysis of estimated radiation doses).	Will be done as part of follow-on to Phase I.
16.	Maurice A. Robkin	Page 19, Table 1	The heading is unclear as written.	Deleted extra word.
17.	MAR	Page 31, lines 1-2	Why is the resulting concentration on the domain boundary nearest the mountains an upper limit?	Revised text to be consistent with PNL-7199 HEDR and PNL-7340 HEDR. Concentrations generally decrease with distance from the source. However, the assumption may not be correct if easterly winds are associated with precipitation, or if the wind patterns near the mountains are curved.
18.	MAR	Page B.7, line 6	Is the following what is meant? Statistical tests based on <u>normal</u> (Gaussian) statistics should not be applied directly to the ratios?	Yes.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
19.	MAR	Table B.4	There are two sets of data given. Which value is associated with which sigma selection method is not clearly given.	See caption for Table B.3.
20.	MAR	Page B.8, line 1	What is the meaning of the "origin" of a log-log plot? The variable values at the intersection of the graph axes is arbitrary depending on the range plotted for ordinate and abscissa.	The statement in the appendix is incorrect. It should refer to forcing the constant to be zero (i.e., $\log y = a + b \log x$ with $a = 0$).
21.	MAR	Page B.10, lines 1-2	For those not completely familiar with atmospheric transport, I expect this statement will be puzzling.	Concur. All releases were made in the morning. Surface heating during the day increases the rate of diffusion. Therefore, diffusion at release time will be slower than experienced during transit to the receptor.
22.	MAR	Page B.10, para. 2, line 10	Provide short explanation why the vertical diffusion "should be good" when the vertical profile of the standard deviation of the wind elevation angle is examined.	Diffusion results from turbulence. The standard deviation of wind elevation is a direct measure of turbulence.
23.	MAR	Page B.11, para. 3	Does the reference to use of all data mean that the data set covers more time than is the case for the data set referred to as the "time of release"?	Yes. "Full data" means the data obtained at 15-min intervals between the release time and arrival at the receptors.
24.	MAR	Page B.11, para. 3	What wind direction data set is used for the straight line model?	The wind direction at the release point at the time of release.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
25.	MAR	Page 8.11, para. 3	Direction of transport increases from the "all data" case, through the "time of release" case to the "straight line model" case? Is this a result of decreasing amounts of data or of model deficiencies?	Both.
26.	Glyn G. Caldwell	Page 4, para. 2, line 1	Were studies of model performance done; were they reported to the TSP; how did the model results differ; why were those excluded based on what results; can a table or graph of comparison of each model versus the true be given?	See Section on Model Performance beginning on Page 21. References contain plots of predicted vs. observed values.
27.	GGC	Page 5, para. 1, line 6	"used" should be "use."	Made correction.
28.	GGC	Page 6, para. 2, lines 7-15	Are models being prepared?	Not part of Phase I. Will be addressed following Phase I.
29.	GGC	Page 7, para. 3	Nonsense.	Revised first sentence of paragraph.
30.	GGC	Page 14, para. 4, lines 2-3	Something is missing from sentence.	Fixed sentence.
31.	GGC	Page 15, line 1	Omit one "on."	Deleted extra word.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
32.	GGC	Page 15, para. 2, line 5	"condition" should read "conditions."	Added an "s."
33.	GGC	Page 18, para. 3, line 4	"winds" should read "wind."	Deleted "s".
34.	GGC	Page 18, para. 4, line 5	"of" should read "to."	Made change.
35.	GGC	Page 23, para. 5, line 2	Omit "an" between "take" and "more."	Deleted the "an".
36.	GGC	Page 28, para. 2, line 6	What does the abbreviation "msl" mean, mean sea level?	Yes.
37.	GGC	Page 35, para. 1, line 3	"used" should read "use."	Made correction.
38.	GGC	Page 35, para. 4, line 4	Insert "with" between "associated" and "strong."	Made correction.
39.	GGC	Page A.6, para. 4, lines 4-5	Is adequate quantitative surface contamination data available; if not, will this prohibit meaningful interpretation of model results?	The appendix provides historical information on the predecessor to HEDR model. Improved deposition modeling will be required in HEDR.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
40.	GGC	Page B.4, para. 4, line 7	Should plume rise be neglected; can plume rise be included if it was observed to be more than 1-2 meters?	Plume rise will be added to the HEDR model following Phase I.
41.	GGC	Page C.7, para. 3, line 7	"show" should read "shown."	Correct.
42.	Allan H. Murphy		This reader is left with the feeling that the selection of the MESOI/MESORAD models may have been based largely on familiarity, availability, and (perceived) feasibility rather than on scientific merit.	Significant changes will be needed in any existing model. This selection minimizes the costs to get initial results.
43.	AHM	Page 6	Questions arise as to the feasibility of making more substantial modifications to the MESOI/MESORAD models in the future to accommodate many relevant physical and/or chemical processes.	The models are modular and provide a flexible framework for any required modifications.
44.	AHM		It is essential that more extensive absolute and relative validations of the MESOI/MESORAD models be undertaken in the HEDR Project area.	Extensive model evaluation studies will be undertaken following Phase I.
45.	AHM		Describe the atmospheric modeling alternatives and model selection considerations before discussing the modeling approach actually taken.	The report organization was selected specifically to put the bottom line first.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
46.	Vietchau Nguyen		Given the underlying assumptions of the Lagrangian formulation (which led to the fundamental MESOI Gaussian solution), applicability of the MESOI formulation to the HEDR Project domain must be justified.	All modeling assumptions and formulations are being reevaluated.
47.	VN		The validity of the assumptions of the slender plume approximation needs to be verified for the HEDR project.	The slender plume approximation is not required for puff models.
48.	VN		Further explanation/justification is required for 1) the weighting process used in the calculation of sector-averaged exposure and 2) the assumption of joint probability of wind direction transport into a sector, wind speed and stability class.	The assumptions related to the sector-average model will be reevaluated before a sector-average model is implemented.
49.	VN		The proposed atmospheric modeling approach requires many computational assumptions, which must be shown to be consistent with the basic physics principles and site conditions.	The consistency and appropriateness of the atmospheric model have been reevaluated, and model revisions are being made. Complete model documentation will be prepared.
50.	VN		The slender plume approximation will undoubtedly underestimate the concentration distant from the area covered by the progression of the plume. This underestimation is inherent in the basic formulation of the MESOI code.	This assertion is incorrect as long as concentration predictions are limited to the air near the surface.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
51.	VN		Using the NRC approximation would result in overestimation of concentrations in the near-field and near the puff trajectory and underestimation of values far-field and/or away from the puff trajectory.	Evaluation of methods of calculating diffusion coefficients will occur following Phase I.
52.	VN		The concept of sector averaging, as presented in this report, seems to be arbitrary and has no physical foundation.	The concept is based on the representation of imprecision of recorded wind directions and the probability that the plume center line will be in a specific position.
53.	VN		Due to the rapid chemical reactions of some released radionuclides in the atmosphere, the fundamental principles used by MESOI and the underlying assumptions concerning the advection time scale and the chemical reaction time scale must be reexamined.	Representation of various iodine-131 species will be examined following Phase I.
54.	VN		A computational mechanism must be provided to reconcile all possible errors resulting from the assumptions and approximations made in the atmospheric transport modeling approach using MESOI.	Model sensitivity and uncertainty will be addressed following Phase I.
55.	VN		A brief description of several modeling approaches being looked at by PNL has been discussed. No reference is provided on the theoretical and user's manuals of the codes under consideration. No criteria for the selection process are fully spelled out.	Various models, including the EPA models (MESOPUFF, INPUFF, MITDIS), have been considered.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
56.	VN		No clear and comprehensive documentation of the latest MESOI/MESORAD generation of codes is provided or referenced.	The latest MESOI/MESORAD documentation is referenced. Documentation for MESOILT2 has been published (PNL-7340 HEDR).
57.	VN	Pages 21-25	Comparative studies between different computer codes are not clearly and fully described in the text.	These studies are beyond the scope of this report.
58	VN		Clarification of several statements in the text is necessary. Examples of statements with no justification in regard to HEDR Project follow:	
58a.	VN	Page 4, para. 3	"the Lagrangian puff approach has the edge over the segmented plume approach"	The requested plume and puff approaches are compared on pages 14 through 16.
58b.	VN	Page 4, para. 4	"Consequently the simpler, sector-averaged Gaussian plume approach is the preferred modeling alternative for receptors near the source."	The statement is based on cost and time of the model vs the importance of changes of meteorological conditions in time and space. A Monte Carlo approach with a straight-line model may be even better than the sector-average model.
58c.	VN	Page 5	Second paragraph from bottom: "The performance of the current MESOI/MESORAD is well documented"	See Appendixes B and C; also see Lewellen et al. 1985, Lewellen et al. 1987.
58d.	VN	Page 22, Table 2	MESOI does not appear in the table.	MESOI was not among the models evaluated in 1981.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
59.	VN	Page 27	PNL has failed to show how the site conditions are compatible with all the theoretical assumptions and approximations made in the current MESOI code under study.	The site conditions do not satisfy all assumptions and approximations made in any code.
60.	VN	Pages 35, E.5-E.8	The report describes six wind patterns that are common on the Hanford Site, but shows eight wind vector plots in Appendix E.	Appendix E then identifies the 6 significant patterns in Table E.2.
61.	VN		Appendix A is a poor presentation of the MESOI code. The content has been presented in 1984, and updates currently used by PNL have not been included. No flow chart is shown.	Appendix A was not intended for experts in transport and diffusion, but still describes the basic structure of MESOI. Complete documentation of the HEDR version of the code has been published (PNL-7340 HEDR).
62.	VN		Appendix B requires a detailed description of all steps and a demonstration that the Savannah River Laboratory MATS data may have some similarities to HEDR data, to demonstrate the applicability to the problem at Hanford.	Appendix B describes MESOI performance on one set of data and compares this performance with that of less complex models.
63.	VN		Appendix C: Given the nature of the data available, a dynamical on-line approach which accounts for data and model uncertainty would be more suited than the proposed statistical analysis technique.	Appendix C describes the performance of a version of MESOI in a climatological application. This analysis was not done as part of the HEDR Project. More detailed evaluations of model performance will be conducted following Phase I.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
64.	VN		Appendix D, Derivation of the Straight-Line Gaussian Model needs to be clarified.	Detailed tests can be reviewed if more information is desired.
65.	VN		Appendix E: Though a more detailed description of the results is recommended, the text does not explain how to obtain the joint probability of wind direction transport into a sector, wind speed and stability class.	This appendix was included to illustrate the typical flow patterns. However, the flow patterns have not been incorporated in any model.
66.	VN		Sensitivity analyses should be performed to establish the variations which are inherently allowed by the intrinsic formulation of the code. Sensitivity studies for each sigma-2 parameterization is also recommended.	Sensitivity and uncertainty studies will be performed following Phase I.
67.	VN		All sigma-2 parameterizations should be tested and compared against data and against each other.	See comment 66.
68.	VN		Because of the inadequate knowledge of the performance of model parameters at larger spatial scale, radionuclide concentrations (near and far-field) should be computed for a given probability and confidence level addressing different types of uncertainty.	Model sensitivity and uncertainty will be addressed following Phase I.
69.	John E. Till	Page 3, para. 2	Add comments explaining why "no existing model was entirely satisfactory."	Added sentence to text.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
70.	JET	Page 4, para. 2, line 4	Beginning with "Considering that the...." I do not understand the sentence.	Revised text to clarify.
71.	JET	Page 4, para. 3, line 6	"approach involves a number <u>of</u> other considerations."	Added "of."
72.	JET		The descriptions of the models are fine. The addition of figures would greatly enhance the presentation.	Figures are not readily available for models other than a puff model.
73.	JET	Page 22, Table 2	Add footnotes defining R_m , R_w , R_{10} .	Added definitions.
74.	JET	Page 23, para. 5, line 2	"They take more than...."	Corrected.
75.	JET	Page 30, Figure 2	A better explanation is needed, along with support of the TSP, for shifting the 10-county area to the east.	Substituted paragraph from PNL-7340 HEDR. Domain location was discussed with TSP prior to the Phase I calculations.
76.	JET	Page 31	Hanford Data: PNL-7199 stated that we did not have the met data for 1944-47. Do we have this met data or not? If we have it, when did we get it and why has it not been keyed in?	PNL-7199 says that the pre-1955 HMS data were available only in paper form at the beginning of the HEDR Project and that the data through 1949 have been entered in the data base. The met data for surrounding stations were received too late for use in the Phase I

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
77.	JET	Page 37, para. 2	To validate these statements, list the periods (for 1944-1947) for which we have data, e.g., on what periods are covered by hourly, daily, weekly, monthly, and quarterly estimates of the source term.	calculations. All 1944-1947 wind data have been entered into the data base. The information on source terms improved significantly in 1991. We now have data to identify days with releases and can generally narrow release times to within one of two shifts.
78.	JET		The report needs a conclusion.	The conclusions are presented in the section following the introduction.
79.	JET		Difficult to determine what is new work and what was done prior to the project beginning. Are Appendices C and D new work? Appendix E lists authors but not where the work was presented.	Appendixes A, B, and C are old work. Appendix D is new, but not original. A footnote was added to Appendix E.
80.	JET		Example printouts of the code should be included in an appendix along with information about how to use the MESOI model.	Beyond the scope of the report. Complete code documentation has been published for the MESOILT2 code used in the Phase I calculations (PNL-7340 HEDR).
81.	Richard L. Morrill		It is a big pain to read reports bound with 1 staple in the upper corner. Please bind them along the side as in the milk report. I appreciated the discussion and evaluation of modelling alternatives. But these documents are	The request will be considered for future reports. Full descriptions of model parameters for Phase I are included

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
82.	RLM	Page 4	short on detail (for example, should provide typical horizontal and vertical diffusion coefficients, their typical range and why). When are we going to get a report on the wet and dry deposition component of the model? I feel incomplete without it.	in PNL-7340 HEDR. Descriptions including ranges will be provided in future reports. The wet and dry deposition components of the model are described in PNL-7340 HEDR.
83.	RLM	Pages 5, 35	Are the 6 wind patterns strictly local or do they apply to the broader area? Hasn't Battelle derived typical wind patterns for the larger study rectangle? If not, why not?	The patterns are based on data collected using the Hanford Telemetry System - wind patterns for the full model domain haven't been requested.
84.	RLM	Page 6	It is noted that the model "should" be modified to permit other parameters to vary spatially. Which parameters? Precipitation? Temperature? Hasn't any of this been done?	Added explanation. The addition of spatial variation of stability, etc., has been discussed for several years but hasn't been done.
85.	RLM	Page 7	What kinds of "different parameterization" are going to be evaluated?	Modified text.
86.	RLM	Page 30	The offsetting of the model domain to the east is very sensible and realistic, but if so, let's get some output for a few places on the eastern edge, like Pullman and Spokane. Presumably the model generated them.	Air concentrations, etc., for the eastern boundary have been computed to be used in discussions of models with the TSP. However, doses have not been calculated for these areas. Presentation of results is beyond the scope of this report.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
87.	RLM	Page 37	Are records really so bad that major unplanned releases were not pinned down by time? I don't believe it.	The records are incomplete.
88.	RLM	Page A.3	I see no justification for failure to incorporate known variability in temperature and precipitation within the study domain into the model, if wet and dry deposition differ.	Appendix A is a general description of MESOI prepared in 1984. Incorporation of spatial variability in precipitation, etc., was not appropriate for model applications at that time. Such variability will be added to the model.
89.	J. Stohr	Page 4, para. 3, line 6	The word "of" is missing.	Added "of."
90.	JS		When does Battelle suggest that the model be changed to allow all meteorological conditions to vary with position in the model domain? What is the maximum expected, or typical difference that these changes will produce in estimates?	Modifications of this sort should be made following Phase I. These modifications are not likely to make large differences in annual doses.
91.	JS		What is Battelle's recommendation for when the other model development issues identified should be addressed? It would be useful to have more information on how much effort would be expended to produce a given improvement in the results.	Phase I is intended to demonstrate that the suggested approach is feasible and practical. Major model development should not be started until the Phase I results have been analyzed.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
92.	B. Shleien		Need sensitivity and uncertainty analyses which would provide assurance that the Phase I results will stand up to future scrutiny.	Sensitivity and uncertainty analyses are scheduled following Phase I.
93.	BS		There is a factor of two difference in the GENII code due to an interface error in the met portion of the model. However, the Phase I results for the HEDR project by-pass the GENII met model.	GENII and the HEDR atmospheric model are only distantly related. Errors in GENII are unrelated to the HEDR atmospheric model.
94.	M. A. Robkin	Page 13	The comment that the assumption of a random release is adequate to justify the sector average model needs more explanation.	Added text.
95.	MAR	Page 16	The word "of" is left out on the first line--centers (of) puffs.	Added "of."
96.	MAR	Page 16	A little more detailed explanation of the phrase "disconnected plume segments" would be useful. Why talk about plumes at all since they imply x-direction integration?	Revised text - we are using a sequence of puffs to represent a plume. X-direction integration is not required to visualize a real plume.
97.	MAR	Page 16, para. 3, line 2	The word "by" is omitted--models (by) summation	Added "by."
98.	MAR	Page 16, para. 3, line 3	accurate(ly).	Changed.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
99.	MAR	Page 19, Table 1	Heading as written is very unclear. It looks like words are omitted or wrong word(s) used.	Deleted extra word.
100.	MAR	Pages 22-23	The definitions of Rm, Rw, and R10 would be better placed at the bottom of the table instead of on the next page. The definition should include what is being correlated with what.	Added footnote.
101.	MAR	Page 31	Top of the page: does the presence of mountainous areas outside the transport domain affect the domain actually used? Can their effects be neglected even if outside the domain?	Revised paragraph for consistency with PNL-7199 HEDR and PNL-7340 HEDR - The mountains were one factor considered in selecting the domain location.
102.	MAR	Page 31, lines 1-2	Is neglecting the effects of hills and mountains what is meant?	No - The model does not incorporate appropriate physics to account for the effects of mountains.
103.	MAR	Pages 8.9, B.10	More explanation is needed as to why atmospheric stability is expected to decrease and the mixing layer to increase as the effluent is transported to the samplers.	See comment 21.
104.	MAR	Pages 8.9, B.10	What is mean by "the vertical diffusion should be good to at least 300 m"? What does "good" mean in this context?	See comment 22.

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Comment Number	Commenter	Page, Paragraph	Comment Summary	Resolution
105.	MAR	Page B.11	The difference between average direction error and average error magnitude is not clear. What is the explicit definition of these quantities?	Average direction error is $1/N \sum \Delta\theta$ where N is number of observations with $\Delta\theta = \theta_p - \theta_o$ where θ_p is predicted direction and θ_o is observed direction. The average error magnitude is $1/N \sum \Delta\theta $.

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18 Technical Steering Panel

D. S. Barth
University of Nevada
4505 Maryland Parkway
Las Vegas, NV 89154

W. A. Bishop
2503 Wedgewood Court SE
Olympia, WA 98501

M. L. Blazek
Oregon Department of Energy
625 Marion Street N.E.
Salem, OR 97310

G. G. Caldwell
Director
Tulsa City-County Health Dept
4616 East 15th Street
Tulsa, OK 74112

S. N. Davis
Dept. of Hydrology & Water
Resources
Bldg. 11
University of Arizona
Tucson, AZ 85721

N. J. Germond
224 Iron Mountain Blvd.
Lake Oswego, OR 97034

P. C. Klingeman
Civil Engineering Dept.
Oregon State University
Corvallis, OR 97331-2302

K. J. Kopecky
Fred Hutchinson Cancer
Research Center
1124 Columbia Street
Seattle, WA 98104

R. L. Morrill
Dept. of Geography
DP-10
University of Washington
Seattle, WA 98195

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